



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:58 AM UTC

PDB ID : 8XA1 / pdb_00008xa1
EMDB ID : EMD-38191
Title : Portal vertex capsomer of VZV B-capsid
Authors : Nan, W.; Lei, C.; Xiangxi, W.
Deposited on : 2023-12-01
Resolution : 4.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

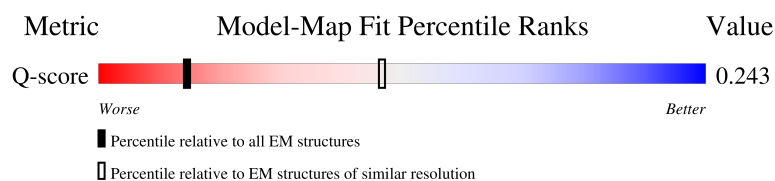
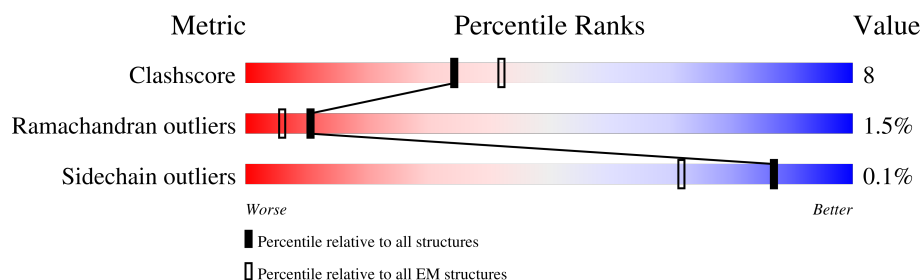
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1345	
2	C	1297	
3	G	297	
3	I	297	

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Mol	Chain	Length	Quality of chain
4	P	307	61% 68% 27%
4	R	307	40% 72% 25%
5	Y	357	27% 59% 22% 19%
5	d	357	34% 71% 25%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 33981 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1345	Total	C	N	O	S	0	0
			10340	6543	1816	1917	64		

- Molecule 2 is a protein called major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1297	Total	C	N	O	S	0	0
			10033	6354	1760	1856	63		

- Molecule 3 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	297	Total	C	N	O	S	0	0
			2124	1367	365	383	9		
3	I	297	Total	C	N	O	S	0	0
			2124	1367	365	383	9		

- Molecule 4 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	307	Total	C	N	O	S	0	0
			2279	1456	399	413	11		
4	R	307	Total	C	N	O	S	0	0
			2279	1456	399	413	11		

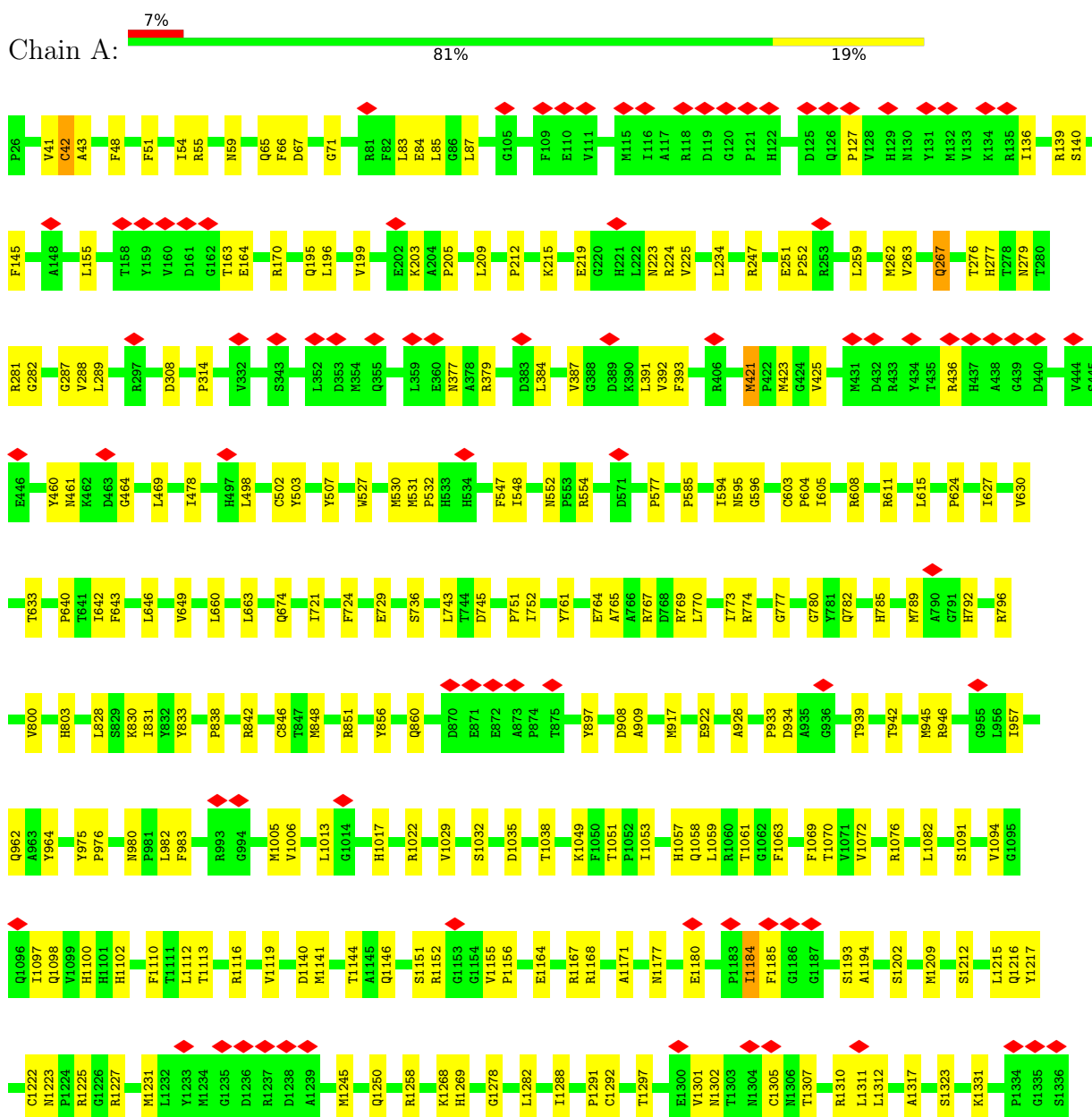
- Molecule 5 is a protein called Tri1.

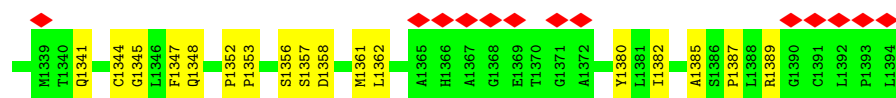
Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	289	Total	C	N	O	S	0	0
			2198	1392	397	395	14		
5	d	357	Total	C	N	O	S	0	0
			2604	1640	475	474	15		

3 Residue-property plots

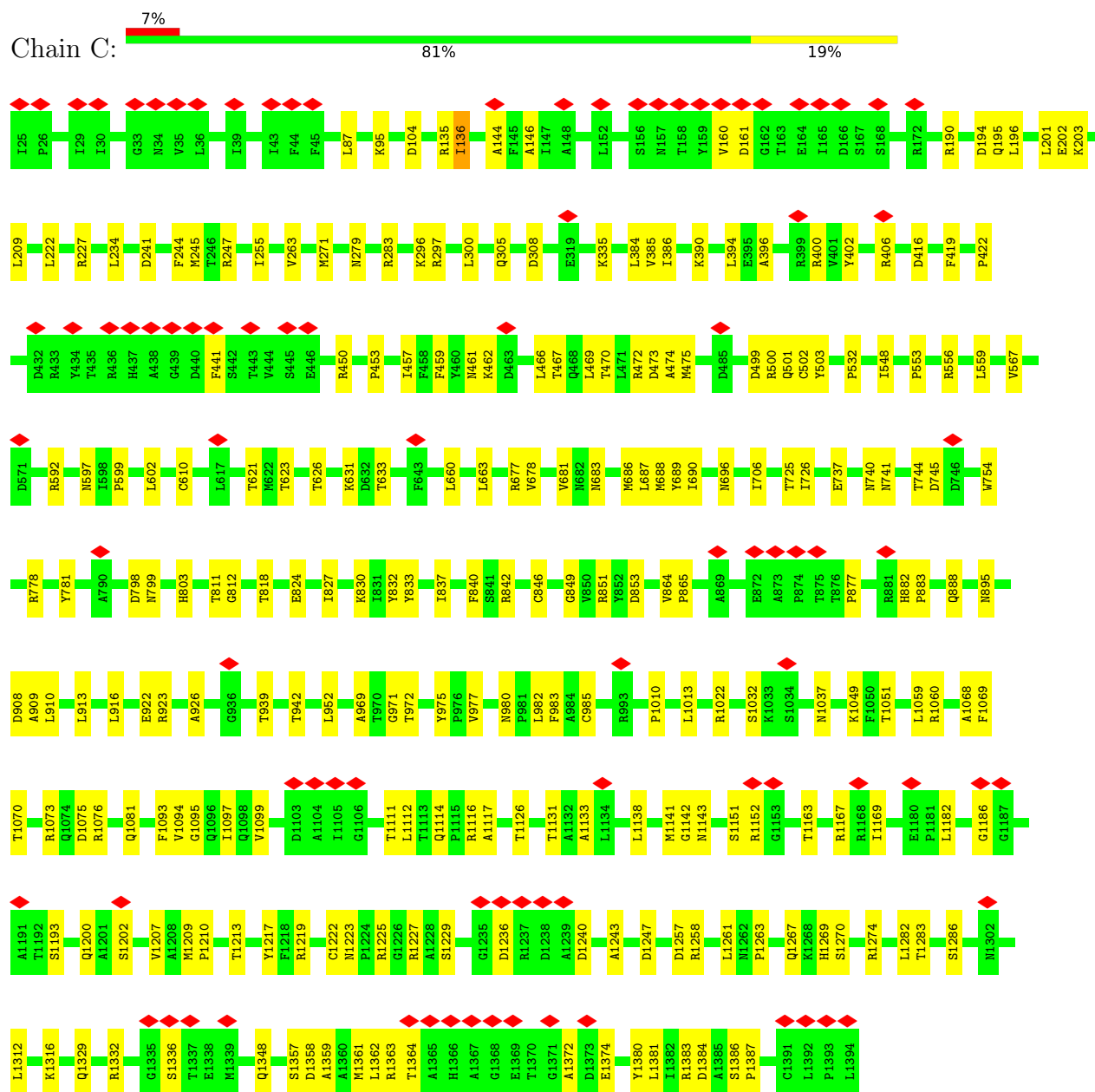
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Major capsid protein

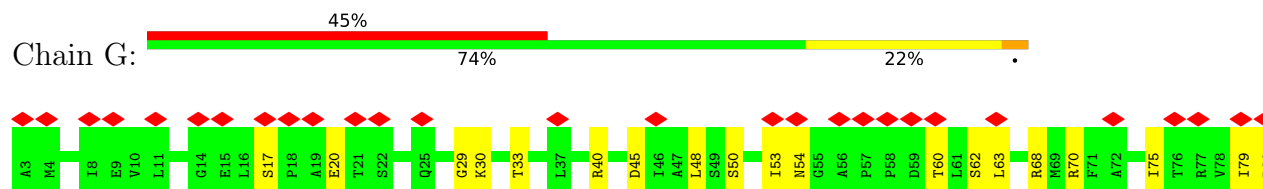


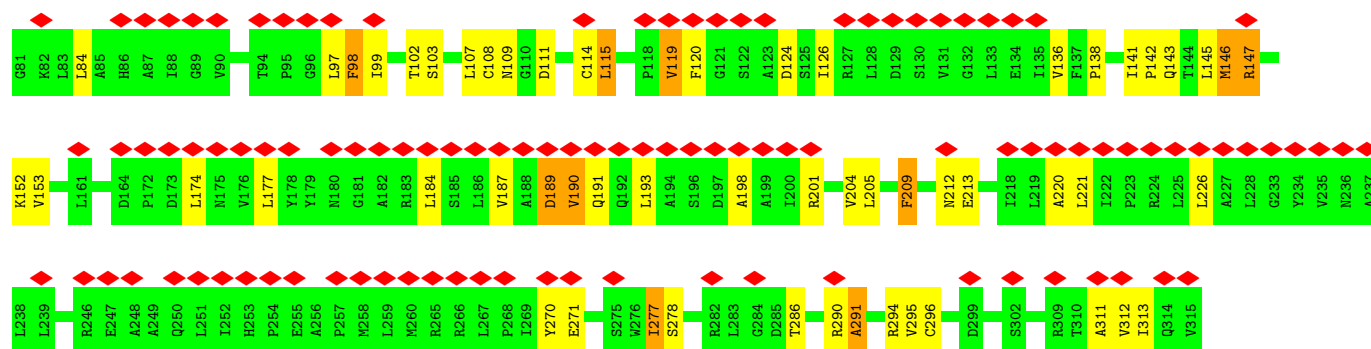


• Molecule 2: major capsid protein

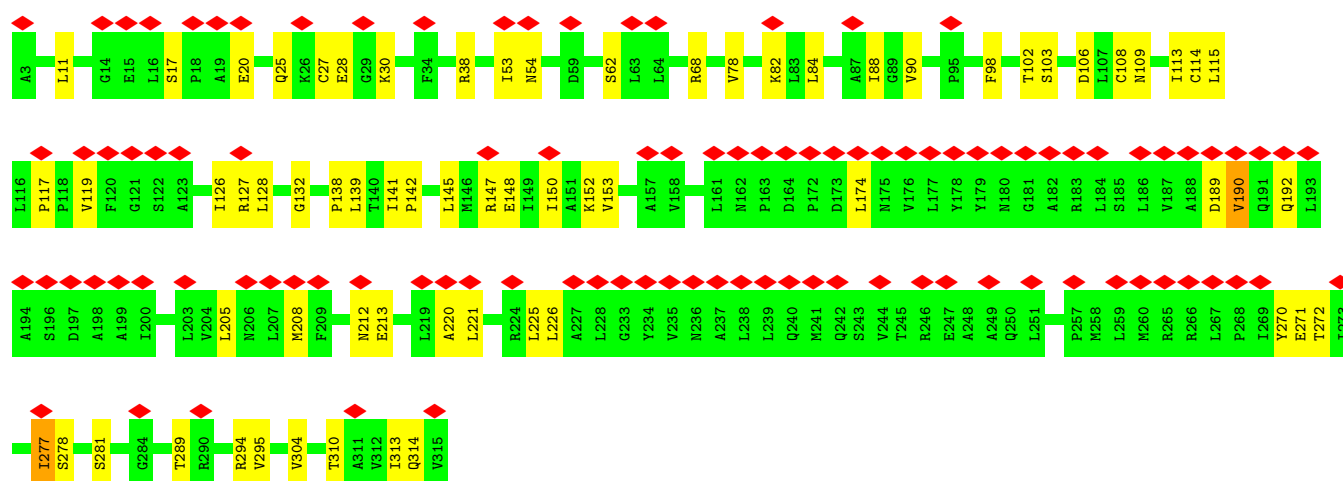
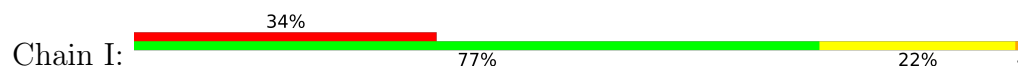


• Molecule 3: Tri2A

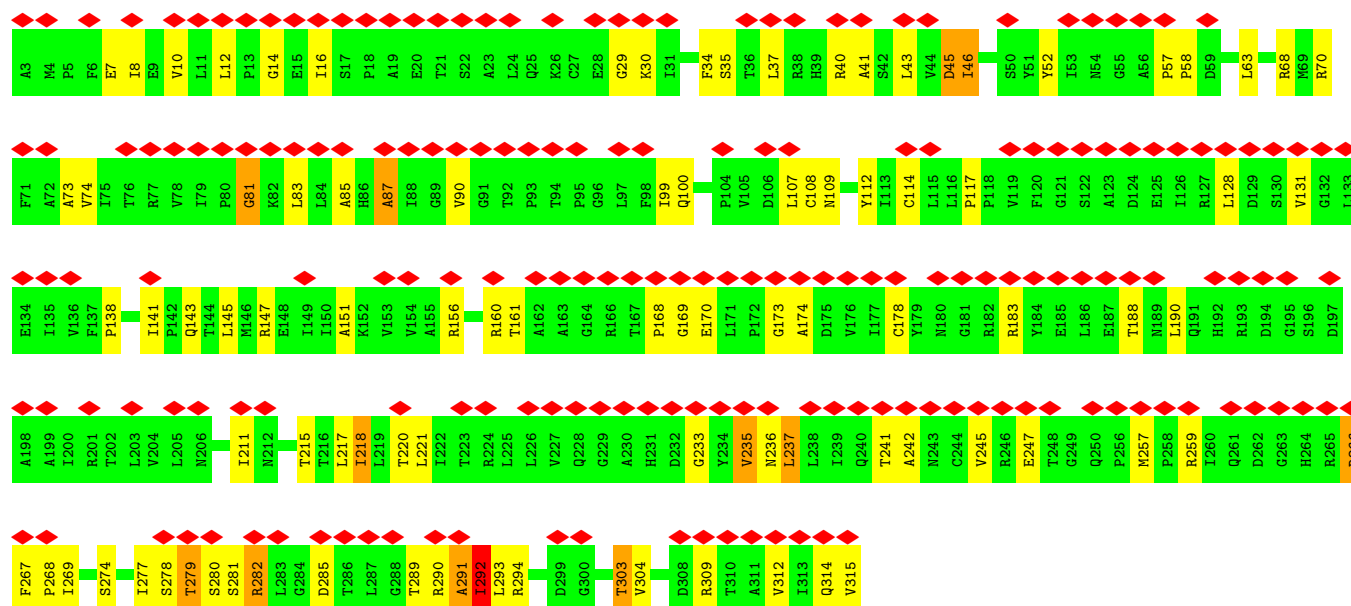




• Molecule 3: Tri2A



• Molecule 4: Tri2B



Chain R:

40% 72% 25%

Chain Y:

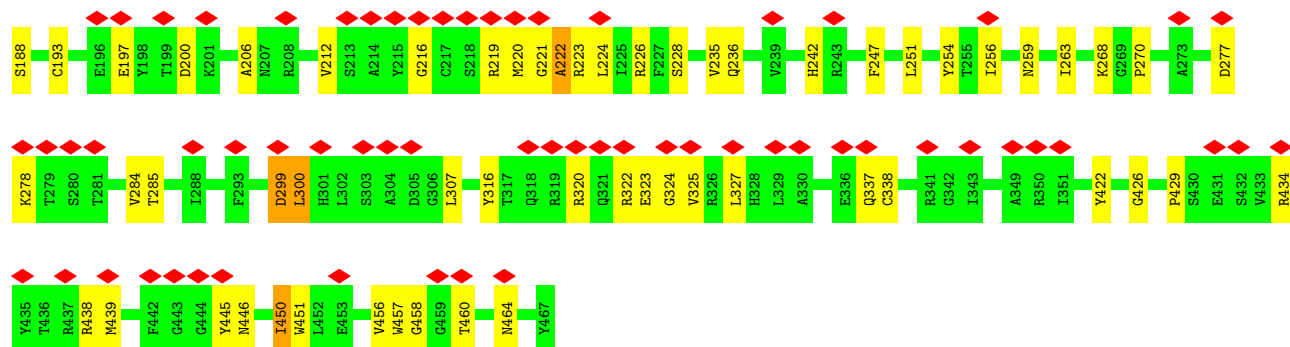
Sequence logo for Chain Y. The y-axis lists amino acids (ALA, ARG, ASP, ASN, CYS, GLN, GLY, ILE, LEU, LYS, MET, PHE, PRO, SER, THR, TRP, VAL). The x-axis shows positions 1 to 20. A bar chart at the top indicates the overall frequency of each amino acid: ALA (27%), ARG (59%), ASP (22%), and ASN (19%).

Chain d:

34% 71% 25% .

Q13 V114 T117 D118 F119 F120 R121 P122 D123 I124 E125 H126 A127 L132 I133 T138 D139 L140 P141 H142 L143 L144 R145 H146 R147 A148 P149 P150 G151 R152 Q153 T154 E155 R156 L157 A158 E159 A160 W161 G162 Q163 L164 L165 E166 A167 S168 E176 S177 G178 A179 R181 A182 Y183 V184 Q187

A8 A9 A10 A11 A12 A13 A14 A15 A16 A17 A18 A19 A20 A21 A22 A23 A24 A25 A26 A29 A30 A31 A36 A44 A45 A46 A47 A48 A49 A76 A77 A78 A79 A82 A83 A84 A85 A86 A87 A88 A89 A90 A91 A99 A100 A101 A102 A103 A104 A105 A106 A107 A108 A109



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.032	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	418.5, 418.5, 418.5	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/10588	0.62	5/14438 (0.0%)
2	C	0.22	0/10275	0.58	2/14009 (0.0%)
3	G	0.31	0/2158	0.96	18/2951 (0.6%)
3	I	0.30	0/2158	0.90	10/2951 (0.3%)
4	P	0.32	0/2320	1.00	28/3165 (0.9%)
4	R	0.30	0/2320	0.97	24/3165 (0.8%)
5	Y	0.31	0/2244	0.92	9/3050 (0.3%)
5	d	0.38	0/2651	1.12	34/3612 (0.9%)
All	All	0.27	0/34714	0.78	130/47341 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	2
3	G	0	3
3	I	0	3
4	P	0	4
4	R	0	3
5	d	0	4
All	All	0	20

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	291	ALA	CA-C-N	11.38	142.18	121.70
4	P	291	ALA	C-N-CA	11.38	142.18	121.70
3	G	277	ILE	CA-C-N	10.28	140.20	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	277	ILE	C-N-CA	10.28	140.20	121.70
3	I	277	ILE	CA-C-N	9.91	139.53	121.70
3	I	277	ILE	C-N-CA	9.91	139.53	121.70
5	Y	450	ILE	CA-C-N	9.56	138.91	121.70
5	Y	450	ILE	C-N-CA	9.56	138.91	121.70
5	d	450	ILE	CA-C-N	9.35	138.54	121.70
5	d	450	ILE	C-N-CA	9.35	138.54	121.70
3	I	270	TYR	CA-C-N	8.80	137.54	121.70
3	I	270	TYR	C-N-CA	8.80	137.54	121.70
5	Y	299	ASP	CA-C-N	8.25	136.56	121.70
5	Y	299	ASP	C-N-CA	8.25	136.56	121.70
3	G	270	TYR	CA-C-N	8.21	136.49	121.70
3	G	270	TYR	C-N-CA	8.21	136.49	121.70
4	P	14	GLY	CA-C-N	8.14	136.35	121.70
4	P	14	GLY	C-N-CA	8.14	136.35	121.70
5	d	299	ASP	CA-C-N	8.14	136.35	121.70
5	d	299	ASP	C-N-CA	8.14	136.35	121.70
5	d	29	ALA	CA-C-N	7.80	135.74	121.70
5	d	29	ALA	C-N-CA	7.80	135.74	121.70
5	d	47	ALA	CA-C-N	7.52	135.24	121.70
5	d	47	ALA	C-N-CA	7.52	135.24	121.70
5	d	21	ALA	CA-C-N	7.43	135.08	121.70
5	d	21	ALA	C-N-CA	7.43	135.08	121.70
4	P	161	THR	CA-C-N	7.33	134.90	121.70
4	P	161	THR	C-N-CA	7.33	134.90	121.70
4	R	161	THR	CA-C-N	7.27	134.79	121.70
4	R	161	THR	C-N-CA	7.27	134.79	121.70
4	R	217	LEU	CA-C-N	7.25	135.03	121.97
4	R	217	LEU	C-N-CA	7.25	135.03	121.97
5	Y	221	GLY	CA-C-N	7.19	134.64	121.70
5	Y	221	GLY	C-N-CA	7.19	134.64	121.70
4	R	14	GLY	CA-C-N	7.09	134.47	121.70
4	R	14	GLY	C-N-CA	7.09	134.47	121.70
5	Y	188	SER	N-CA-C	-7.07	106.56	114.62
3	G	115	LEU	CA-C-N	6.99	131.31	120.68
3	G	115	LEU	C-N-CA	6.99	131.31	120.68
4	P	170	GLU	CA-C-N	6.97	134.24	121.70
4	P	170	GLU	C-N-CA	6.97	134.24	121.70
4	P	45	ASP	CA-C-N	6.87	134.34	121.97
4	P	45	ASP	C-N-CA	6.87	134.34	121.97
4	R	179	TYR	CA-C-N	6.83	134.58	121.54
4	R	179	TYR	C-N-CA	6.83	134.58	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	14	ALA	CA-C-N	6.68	133.73	121.70
5	d	14	ALA	C-N-CA	6.68	133.73	121.70
4	R	45	ASP	CA-C-N	6.66	133.95	121.97
4	R	45	ASP	C-N-CA	6.66	133.95	121.97
5	d	16	ALA	CA-C-N	6.55	133.50	121.70
5	d	16	ALA	C-N-CA	6.55	133.50	121.70
5	d	434	ARG	CA-C-N	6.55	133.49	121.70
5	d	434	ARG	C-N-CA	6.55	133.49	121.70
3	G	209	PHE	CA-C-N	6.45	133.31	121.70
3	G	209	PHE	C-N-CA	6.45	133.31	121.70
4	R	170	GLU	CA-C-N	6.26	132.97	121.70
4	R	170	GLU	C-N-CA	6.26	132.97	121.70
3	G	62	SER	CA-C-N	6.23	132.92	121.70
3	G	62	SER	C-N-CA	6.23	132.92	121.70
1	A	59	ASN	N-CA-C	6.08	117.39	108.14
4	R	247	GLU	CA-C-N	6.04	135.64	125.02
4	R	247	GLU	C-N-CA	6.04	135.64	125.02
4	P	277	ILE	CA-C-N	6.01	133.02	121.54
4	P	277	ILE	C-N-CA	6.01	133.02	121.54
3	G	102	THR	CA-C-N	6.01	136.47	121.80
3	G	102	THR	C-N-CA	6.01	136.47	121.80
5	d	221	GLY	CA-C-N	5.92	132.36	121.70
5	d	221	GLY	C-N-CA	5.92	132.36	121.70
1	A	421	MET	CG-SD-CE	5.90	113.89	100.90
3	I	62	SER	CA-C-N	5.90	132.32	121.70
3	I	62	SER	C-N-CA	5.90	132.32	121.70
3	I	102	THR	CA-C-N	5.89	136.18	121.80
3	I	102	THR	C-N-CA	5.89	136.18	121.80
4	R	237	LEU	CA-C-N	5.83	132.20	121.70
4	R	237	LEU	C-N-CA	5.83	132.20	121.70
5	Y	434	ARG	CA-C-N	5.78	132.11	121.70
5	Y	434	ARG	C-N-CA	5.78	132.11	121.70
4	P	87	ALA	CA-C-N	5.78	132.10	121.70
4	P	87	ALA	C-N-CA	5.78	132.10	121.70
4	R	268	PRO	CA-C-N	5.71	132.25	121.97
4	R	268	PRO	C-N-CA	5.71	132.25	121.97
2	C	1312	LEU	CA-C-N	-5.69	112.09	122.38
2	C	1312	LEU	C-N-CA	-5.69	112.09	122.38
5	d	88	PRO	CA-C-N	5.68	131.92	121.70
5	d	88	PRO	C-N-CA	5.68	131.92	121.70
4	P	268	PRO	CA-C-N	5.67	132.17	121.97
4	P	268	PRO	C-N-CA	5.67	132.17	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	247	GLU	CA-C-N	5.63	136.42	126.45
4	P	247	GLU	C-N-CA	5.63	136.42	126.45
4	R	96	GLY	N-CA-C	5.63	129.62	113.30
4	R	266	ARG	CA-C-N	5.62	131.81	121.70
4	R	266	ARG	C-N-CA	5.62	131.81	121.70
4	P	217	LEU	CA-C-N	5.59	132.03	121.97
4	P	217	LEU	C-N-CA	5.59	132.03	121.97
5	d	17	ALA	CA-C-N	5.56	131.71	121.70
5	d	17	ALA	C-N-CA	5.56	131.71	121.70
3	G	189	ASP	CA-C-N	5.55	131.96	121.97
3	G	189	ASP	C-N-CA	5.55	131.96	121.97
4	R	87	ALA	CA-C-N	5.55	131.68	121.70
4	R	87	ALA	C-N-CA	5.55	131.68	121.70
1	A	71	GLY	CA-C-N	5.52	130.66	122.82
1	A	71	GLY	C-N-CA	5.52	130.66	122.82
3	I	189	ASP	CA-C-N	5.48	131.84	121.97
3	I	189	ASP	C-N-CA	5.48	131.84	121.97
4	P	266	ARG	CA-C-N	5.48	131.57	121.70
4	P	266	ARG	C-N-CA	5.48	131.57	121.70
5	d	46	ALA	CA-C-N	5.46	131.96	121.54
5	d	46	ALA	C-N-CA	5.46	131.96	121.54
5	d	242	HIS	CA-C-N	5.43	131.91	121.54
5	d	242	HIS	C-N-CA	5.43	131.91	121.54
3	G	119	VAL	N-CA-C	-5.42	98.07	109.34
5	d	76	ILE	CA-C-N	5.39	131.68	121.97
5	d	76	ILE	C-N-CA	5.39	131.68	121.97
4	P	81	GLY	CA-C-N	5.36	131.79	121.54
4	P	81	GLY	C-N-CA	5.36	131.79	121.54
4	P	292	ILE	N-CA-CB	5.33	120.57	111.50
5	d	108	THR	CA-C-N	5.24	131.14	121.70
5	d	108	THR	C-N-CA	5.24	131.14	121.70
4	P	237	LEU	CA-C-N	5.18	131.03	121.70
4	P	237	LEU	C-N-CA	5.18	131.03	121.70
4	P	282	ARG	CA-CB-CG	5.15	124.40	114.10
4	R	282	ARG	CA-CB-CG	5.15	124.39	114.10
5	d	323	GLU	CA-C-N	5.14	130.96	121.70
5	d	323	GLU	C-N-CA	5.14	130.96	121.70
1	A	1184	ILE	CG1-CB-CG2	-5.13	95.31	110.70
3	G	147	ARG	CA-CB-CG	5.05	124.20	114.10
3	G	97	LEU	CA-C-N	5.02	131.13	121.54
3	G	97	LEU	C-N-CA	5.02	131.13	121.54
5	d	22	ALA	CA-C-N	5.02	130.73	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	d	22	ALA	C-N-CA	5.02	130.73	121.70

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	LEU	Peptide
2	C	136	ILE	Peptide
2	C	202	GLU	Peptide
3	G	146	MET	Peptide
3	G	209	PHE	Peptide
3	G	271	GLU	Peptide
3	I	108	CYS	Peptide
3	I	271	GLU	Peptide
3	I	272	THR	Peptide
4	P	145	LEU	Peptide
4	P	151	ALA	Peptide
4	P	290	ARG	Peptide
4	P	81	GLY	Peptide
4	R	151	ALA	Peptide
4	R	218	ILE	Peptide
4	R	292	ILE	Peptide
5	d	107	THR	Peptide
5	d	220	MET	Peptide
5	d	222	ALA	Peptide
5	d	438	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10340	0	10012	152	0
2	C	10033	0	9816	149	0
3	G	2124	0	2111	45	0
3	I	2124	0	2111	35	0
4	P	2279	0	2316	60	0
4	R	2279	0	2316	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	2198	0	2124	46	0
5	d	2604	0	2521	47	0
All	All	33981	0	33327	545	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (545) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:592:ARG:HH22	2:C:599:PRO:HD3	1.54	0.72
4:P:74:VAL:HG21	4:P:99:ILE:HG22	1.72	0.71
4:R:63:LEU:HD23	4:R:117:PRO:HB3	1.72	0.70
1:A:848:MET:HG3	1:A:976:PRO:HA	1.74	0.69
4:P:63:LEU:HD23	4:P:117:PRO:HB3	1.75	0.69
1:A:926:ALA:HB1	1:A:1013:LEU:HD21	1.75	0.68
5:d:79:ASN:H	5:d:83:ASN:HD21	1.43	0.67
1:A:770:LEU:HB2	1:A:946:ARG:HH12	1.59	0.66
3:I:106:ASP:HB2	3:I:304:VAL:HB	1.77	0.66
2:C:1151:SER:HB2	2:C:1286:SER:HB2	1.78	0.65
2:C:305:GLN:HE21	2:C:386:ILE:HG23	1.61	0.65
1:A:640:PRO:HG3	2:C:696:ASN:HD21	1.62	0.64
4:P:160:ARG:HD3	4:P:190:LEU:HD22	1.78	0.64
1:A:421:MET:HE3	1:A:1353:PRO:HD2	1.79	0.63
3:I:114:CYS:HB3	3:I:138:PRO:HB2	1.81	0.63
1:A:595:ASN:HD21	1:A:611:ARG:HH22	1.45	0.63
5:d:439:MET:HE1	5:d:446:ASN:HD21	1.62	0.63
4:P:8:ILE:HB	4:P:85:ALA:HB3	1.80	0.63
5:Y:195:ALA:HB3	5:Y:208:ARG:HE	1.64	0.63
2:C:472:ARG:HA	2:C:1059:LEU:HD13	1.81	0.62
5:d:156:ARG:HH12	5:d:236:GLN:HB2	1.64	0.62
1:A:605:ILE:HD11	1:A:1032:SER:HB2	1.82	0.62
2:C:1068:ALA:HB3	2:C:1209:MET:O	1.99	0.62
1:A:139:ARG:HE	1:A:140:SER:H	1.47	0.62
5:Y:272:GLU:HG3	5:Y:285:THR:HA	1.80	0.62
5:d:316:TYR:H	5:d:325:VAL:HG13	1.63	0.62
4:R:6:PHE:HB3	4:R:87:ALA:HB2	1.82	0.62
1:A:247:ARG:HH22	1:A:1389:ARG:HD2	1.63	0.61
1:A:838:PRO:HB3	1:A:982:LEU:HD21	1.80	0.61
4:P:108:CYS:SG	4:P:109:ASN:N	2.70	0.61
1:A:1184:ILE:HB	4:P:237:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:97:LEU:HB2	4:R:312:VAL:HB	1.82	0.61
2:C:144:ALA:HA	2:C:1111:THR:HA	1.83	0.61
1:A:1216:GLN:HE22	2:C:466:LEU:HB2	1.63	0.61
2:C:660:LEU:HD23	2:C:663:LEU:HD13	1.82	0.61
4:P:107:LEU:HB3	4:P:304:VAL:HB	1.82	0.61
5:Y:323:GLU:HG3	5:Y:324:GLY:HA2	1.82	0.61
4:R:282:ARG:NH2	5:d:464:ASN:OD1	2.34	0.60
5:Y:420:ALA:HB3	5:Y:466:CYS:HB2	1.83	0.60
3:G:205:LEU:HD22	4:P:235:VAL:HG22	1.83	0.60
5:Y:284:VAL:HG13	5:Y:285:THR:HG23	1.83	0.60
2:C:502:CYS:HB2	2:C:532:PRO:HD2	1.83	0.60
3:G:177:LEU:HB2	3:G:184:LEU:O	2.02	0.60
1:A:1005:MET:HG3	1:A:1006:VAL:HG23	1.83	0.60
1:A:308:ASP:HB3	1:A:384:LEU:HD12	1.83	0.60
4:P:211:ILE:HG12	4:P:215:THR:HG21	1.83	0.60
1:A:155:LEU:HA	1:A:170:ARG:HE	1.66	0.60
2:C:459:PHE:O	2:C:466:LEU:HA	2.01	0.60
1:A:980:ASN:HB3	1:A:983:PHE:H	1.67	0.60
2:C:422:PRO:HA	2:C:1070:THR:HG22	1.84	0.60
4:P:35:SER:HB2	4:P:70:ARG:HG2	1.84	0.60
4:P:220:THR:O	4:P:221:LEU:N	2.35	0.59
5:d:219:ARG:NH1	5:d:222:ALA:O	2.34	0.59
2:C:1094:VAL:HA	2:C:1116:ARG:HE	1.67	0.59
2:C:824:GLU:HA	2:C:827:ILE:HG12	1.83	0.59
2:C:1093:PHE:HB2	2:C:1117:ALA:HB3	1.84	0.59
3:G:45:ASP:O	3:G:70:ARG:NH2	2.36	0.59
4:P:108:CYS:HA	4:P:303:THR:HA	1.84	0.59
4:R:208:MET:HA	4:R:211:ILE:HB	1.84	0.59
4:P:68:ARG:O	5:Y:337:GLN:NE2	2.36	0.59
2:C:745:ASP:O	2:C:830:LYS:NZ	2.36	0.59
1:A:1223:ASN:ND2	1:A:1348:GLN:O	2.36	0.59
5:Y:289:PRO:HA	5:Y:451:TRP:H	1.68	0.58
1:A:1168:ARG:HH12	1:A:1180:GLU:HA	1.68	0.58
2:C:1097:ILE:HD11	2:C:1112:LEU:HB3	1.84	0.58
5:d:284:VAL:HG23	5:d:285:THR:HG23	1.86	0.58
3:G:212:ASN:ND2	4:P:218:ILE:O	2.36	0.58
5:d:113:GLN:NE2	5:d:114:VAL:O	2.36	0.58
4:P:257:MET:HE3	4:P:259:ARG:HB2	1.86	0.58
2:C:501:GLN:HB3	2:C:567:VAL:HG11	1.85	0.58
3:G:205:LEU:HD13	4:P:235:VAL:HA	1.85	0.58
1:A:615:LEU:HD21	1:A:1063:PHE:HE1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:279:ASN:HD21	2:C:283:ARG:HB3	1.68	0.58
3:G:111:ASP:HB3	3:G:291:ALA:HB1	1.86	0.58
3:I:68:ARG:O	4:R:294:ARG:NH2	2.37	0.58
3:I:109:ASN:OD1	3:I:294:ARG:NH2	2.36	0.57
1:A:281:ARG:NH1	1:A:308:ASP:OD2	2.38	0.57
2:C:737:GLU:HG3	2:C:744:THR:HG21	1.86	0.57
2:C:247:ARG:NH1	2:C:1387:PRO:O	2.38	0.57
3:G:60:THR:HA	3:G:63:LEU:HD12	1.86	0.57
4:P:10:VAL:HG22	4:P:41:ALA:HB3	1.86	0.57
1:A:1323:SER:OG	1:A:1331:LYS:O	2.22	0.57
4:R:10:VAL:HG13	4:R:83:LEU:HB3	1.86	0.57
4:P:34:PHE:HD2	4:P:37:LEU:HD23	1.70	0.57
5:d:85:GLN:HG2	5:d:91:ILE:HD12	1.86	0.57
2:C:626:THR:HG22	2:C:706:ILE:HG12	1.87	0.57
3:G:187:VAL:HG12	3:G:189:ASP:H	1.70	0.57
4:R:141:ILE:HD11	4:R:145:LEU:HD22	1.87	0.57
5:Y:317:THR:O	5:Y:320:ARG:NH2	2.37	0.57
2:C:631:LYS:NZ	2:C:840:PHE:O	2.37	0.56
1:A:1053:ILE:O	1:A:1057:HIS:ND1	2.36	0.56
1:A:1345:GLY:O	1:A:1348:GLN:NE2	2.38	0.56
5:d:206:ALA:HA	5:d:445:TYR:HE2	1.71	0.56
1:A:774:ARG:NH2	1:A:777:GLY:O	2.39	0.56
1:A:1231:MET:HG3	1:A:1301:VAL:HG21	1.86	0.56
2:C:592:ARG:NH2	2:C:597:ASN:O	2.39	0.56
3:G:152:LYS:HE3	3:G:174:LEU:HD22	1.88	0.56
3:G:17:SER:OG	3:G:20:GLU:OE1	2.23	0.56
4:R:82:LYS:NZ	4:R:83:LEU:O	2.39	0.56
4:P:87:ALA:HB1	4:P:90:VAL:HB	1.87	0.56
1:A:761:TYR:O	1:A:765:ALA:HB2	2.05	0.56
5:d:26:ALA:HB3	5:d:30:ALA:H	1.69	0.56
2:C:467:THR:OG1	2:C:1143:ASN:ND2	2.38	0.56
1:A:1053:ILE:HG22	1:A:1057:HIS:HE1	1.70	0.56
1:A:1070:THR:HG23	1:A:1209:MET:HG2	1.86	0.56
5:Y:441:ARG:HH22	5:Y:446:ASN:HA	1.70	0.55
2:C:842:ARG:NH1	2:C:1032:SER:O	2.40	0.55
5:d:235:VAL:O	5:d:320:ARG:NH2	2.36	0.55
1:A:289:LEU:HD12	1:A:1082:LEU:HD11	1.89	0.55
1:A:314:PRO:HA	1:A:377:ASN:HA	1.88	0.55
1:A:751:PRO:HD2	1:A:833:TYR:HD1	1.71	0.55
3:G:107:LEU:HD12	5:Y:135:ARG:HE	1.70	0.55
1:A:1167:ARG:HH11	1:A:1168:ARG:HH21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:CYS:O	1:A:1310:ARG:NH2	2.36	0.55
3:I:220:ALA:HB2	3:I:225:LEU:HD13	1.88	0.55
4:P:147:ARG:NH2	4:P:285:ASP:OD1	2.37	0.55
3:G:33:THR:OG1	3:G:70:ARG:NH1	2.40	0.55
4:R:222:ILE:HD12	4:R:249:GLY:HA2	1.89	0.55
5:d:236:GLN:HG2	5:d:320:ARG:HG2	1.88	0.55
2:C:190:ARG:NH1	2:C:400:ARG:O	2.39	0.55
2:C:741:ASN:HB3	2:C:744:THR:HG22	1.89	0.55
3:G:295:VAL:HG12	3:G:312:VAL:HG12	1.88	0.55
2:C:1372:ALA:O	2:C:1383:ARG:NH2	2.40	0.54
4:P:147:ARG:NH2	4:P:289:THR:O	2.38	0.54
2:C:1269:HIS:HD2	2:C:1274:ARG:HD3	1.72	0.54
3:G:198:ALA:HB1	3:G:201:ARG:HH21	1.72	0.54
5:Y:423:THR:HB	5:Y:463:TRP:HB3	1.90	0.54
1:A:729:GLU:O	1:A:736:SER:OG	2.25	0.54
1:A:942:THR:HA	1:A:945:MET:HB3	1.90	0.54
2:C:470:THR:HG23	2:C:472:ARG:H	1.71	0.54
2:C:1374:GLU:OE2	2:C:1383:ARG:NH2	2.38	0.54
2:C:1362:LEU:HD23	2:C:1363:ARG:HH11	1.73	0.54
4:R:107:LEU:HB2	4:R:304:VAL:HB	1.89	0.54
2:C:1060:ARG:HH22	2:C:1169:ILE:HD13	1.72	0.53
4:P:37:LEU:HB2	5:Y:307:LEU:HD13	1.91	0.53
1:A:1076:ARG:NH2	1:A:1323:SER:O	2.41	0.53
4:P:73:ALA:HB1	4:P:85:ALA:HB1	1.90	0.53
2:C:271:MET:SD	2:C:271:MET:N	2.73	0.53
1:A:42:CYS:SG	1:A:43:ALA:N	2.77	0.53
1:A:287:GLY:HA3	1:A:392:VAL:HG12	1.90	0.53
1:A:842:ARG:NH1	1:A:1029:VAL:O	2.41	0.53
2:C:1359:ALA:HB1	2:C:1363:ARG:HH12	1.73	0.53
1:A:548:ILE:HD12	1:A:1258:ARG:HD3	1.90	0.53
1:A:1072:VAL:HG13	1:A:1291:PRO:HG2	1.90	0.53
5:Y:441:ARG:HH22	5:Y:447:VAL:H	1.57	0.53
2:C:1258:ARG:HH22	2:C:1261:LEU:HD12	1.73	0.53
2:C:104:ASP:O	2:C:335:LYS:NZ	2.37	0.53
2:C:952:LEU:HD11	2:C:977:VAL:HG13	1.91	0.53
4:R:107:LEU:HD23	4:R:142:PRO:HG3	1.91	0.53
5:Y:450:ILE:HA	5:Y:451:TRP:HB2	1.91	0.53
1:A:939:THR:N	1:A:942:THR:OG1	2.37	0.52
1:A:1184:ILE:HG22	1:A:1185:PHE:H	1.72	0.52
1:A:1193:SER:OG	1:A:1194:ALA:N	2.40	0.52
4:R:108:CYS:SG	4:R:109:ASN:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:316:TYR:H	5:Y:325:VAL:HG13	1.74	0.52
1:A:594:ILE:HG22	1:A:596:GLY:H	1.73	0.52
4:R:214:GLY:HA3	4:R:272:ALA:HB2	1.90	0.52
4:R:285:ASP:O	5:d:337:GLN:NE2	2.42	0.52
5:Y:268:LYS:HA	5:Y:457:TRP:HB2	1.91	0.52
3:I:27:CYS:SG	3:I:30:LYS:NZ	2.76	0.52
5:Y:196:GLU:HG2	5:Y:197:GLU:HG3	1.91	0.52
2:C:1219:ARG:NH1	2:C:1381:LEU:O	2.37	0.52
4:P:156:ARG:NH1	4:P:188:THR:OG1	2.43	0.52
2:C:865:PRO:HD3	2:C:888:GLN:HG2	1.91	0.52
2:C:450:ARG:NH1	2:C:1358:ASP:OD2	2.43	0.52
3:G:30:LYS:NZ	3:G:124:ASP:OD2	2.40	0.52
3:G:277:ILE:H	3:G:278:SER:HB2	1.74	0.52
5:d:141:PRO:HA	5:d:144:ALA:HB3	1.92	0.52
2:C:1076:ARG:HG2	2:C:1138:LEU:HD12	1.91	0.52
2:C:1210:PRO:O	2:C:1213:THR:OG1	2.27	0.52
1:A:856:TYR:O	1:A:860:GLN:NE2	2.43	0.51
2:C:1073:ARG:NH2	2:C:1142:GLY:O	2.44	0.51
3:G:79:ILE:HD12	3:G:80:PRO:HD2	1.93	0.51
4:R:113:ILE:HB	4:R:293:LEU:HB3	1.93	0.51
2:C:663:LEU:HG	2:C:909:ALA:HB1	1.92	0.51
4:P:30:LYS:NZ	4:P:138:PRO:O	2.34	0.51
2:C:1282:LEU:HG	2:C:1283:THR:HG23	1.91	0.51
5:d:268:LYS:NZ	5:d:458:GLY:O	2.43	0.51
5:d:450:ILE:HA	5:d:451:TRP:HB2	1.92	0.51
1:A:624:PRO:HA	1:A:627:ILE:HG22	1.93	0.51
5:d:216:GLY:O	5:d:223:ARG:NH2	2.44	0.51
2:C:1167:ARG:HD2	2:C:1182:LEU:HD21	1.93	0.51
3:G:68:ARG:O	4:P:294:ARG:NH2	2.44	0.51
3:I:88:ILE:O	3:I:314:GLN:NE2	2.43	0.51
5:d:197:GLU:OE2	5:d:322:ARG:NH1	2.42	0.51
3:G:290:ARG:HH21	4:P:315:VAL:HG12	1.76	0.51
3:I:127:ARG:HH12	3:I:132:GLY:HA2	1.75	0.51
4:R:293:LEU:HD12	4:R:312:VAL:HG11	1.93	0.51
5:Y:210:ALA:HB1	5:Y:443:GLY:HA3	1.92	0.51
1:A:552:ASN:OD1	1:A:554:ARG:NH1	2.43	0.51
1:A:674:GLN:NE2	2:C:696:ASN:O	2.44	0.51
2:C:811:THR:OG1	2:C:812:GLY:N	2.44	0.51
4:P:178:CYS:SG	4:P:183:ARG:NH1	2.84	0.51
1:A:83:LEU:O	1:A:85:LEU:N	2.43	0.50
3:G:114:CYS:HB3	3:G:138:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:GLN:CD	1:A:66:PHE:H	2.20	0.50
3:I:281:SER:HB2	4:R:283:LEU:HG	1.92	0.50
5:d:86:ILE:HD11	5:d:90:SER:HB2	1.93	0.50
2:C:908:ASP:OD1	2:C:908:ASP:N	2.43	0.50
3:G:68:ARG:HE	3:G:286:THR:HA	1.76	0.50
4:P:112:TYR:HB2	4:P:143:GLN:HB2	1.94	0.50
5:Y:422:TYR:OH	5:Y:464:ASN:ND2	2.43	0.50
1:A:288:VAL:HA	1:A:393:PHE:HB2	1.93	0.50
3:G:213:GLU:HB3	4:P:245:VAL:HG22	1.93	0.50
1:A:1278:GLY:H	1:A:1297:THR:HG22	1.76	0.50
5:Y:167:ALA:O	5:Y:219:ARG:NH2	2.45	0.50
1:A:127:PRO:HG3	2:C:146:ALA:HB3	1.93	0.50
2:C:194:ASP:OD1	2:C:402:TYR:OH	2.23	0.50
3:I:147:ARG:HA	3:I:150:ILE:HB	1.93	0.50
2:C:833:TYR:HA	2:C:837:ILE:HD13	1.94	0.50
1:A:48:PHE:CD2	1:A:51:PHE:HB2	2.47	0.49
4:R:229:GLY:HA2	4:R:235:VAL:HG21	1.94	0.49
1:A:1098:GLN:HE21	1:A:1113:THR:HB	1.76	0.49
2:C:1223:ASN:ND2	2:C:1348:GLN:O	2.44	0.49
4:P:99:ILE:O	4:P:309:ARG:NH2	2.45	0.49
5:d:121:ARG:NH2	5:d:123:ASP:OD2	2.41	0.49
1:A:425:VAL:HG11	1:A:1215:LEU:HD13	1.94	0.49
4:P:114:CYS:HA	4:P:291:ALA:HB1	1.94	0.49
1:A:627:ILE:HA	1:A:630:VAL:HG12	1.93	0.49
1:A:1302:ASN:O	1:A:1310:ARG:NH1	2.45	0.49
4:P:7:GLU:HA	4:P:85:ALA:O	2.13	0.49
1:A:1151:SER:OG	1:A:1282:LEU:O	2.31	0.49
2:C:1236:ASP:N	2:C:1236:ASP:OD1	2.45	0.49
1:A:1140:ASP:O	1:A:1202:SER:OG	2.27	0.49
2:C:500:ARG:NH1	2:C:501:GLN:O	2.45	0.49
4:P:99:ILE:HD11	4:P:312:VAL:HG21	1.94	0.49
1:A:630:VAL:HA	1:A:633:THR:HG22	1.95	0.49
1:A:642:ILE:HD11	1:A:897:TYR:HB3	1.95	0.49
1:A:1250:GLN:OE1	2:C:1193:SER:OG	2.30	0.49
4:R:178:CYS:SG	4:R:183:ARG:NH1	2.86	0.48
4:R:291:ALA:HB1	4:R:292:ILE:HB	1.95	0.48
1:A:436:ARG:HH12	2:C:1364:THR:HA	1.78	0.48
2:C:279:ASN:OD1	2:C:283:ARG:N	2.47	0.48
2:C:913:LEU:HA	2:C:916:LEU:HB2	1.95	0.48
2:C:1073:ARG:NH2	2:C:1202:SER:OG	2.42	0.48
3:G:29:GLY:H	3:G:75:ILE:HB	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:d:223:ARG:HG3	5:d:224:LEU:HG	1.95	0.48
1:A:1091:SER:OG	1:A:1119:VAL:O	2.25	0.48
2:C:297:ARG:HA	2:C:300:LEU:HG	1.94	0.48
2:C:201:LEU:O	2:C:1316:LYS:NZ	2.37	0.48
1:A:1344:CYS:HA	1:A:1347:PHE:HB2	1.95	0.48
1:A:1358:ASP:HB3	1:A:1361:MET:HG3	1.96	0.48
5:d:212:VAL:HG12	5:d:223:ARG:HD2	1.95	0.48
1:A:604:PRO:HG3	1:A:1212:SER:HB2	1.95	0.48
1:A:1307:THR:HG22	1:A:1311:LEU:HD23	1.95	0.48
2:C:1332:ARG:NH2	2:C:1336:SER:O	2.39	0.48
3:I:115:LEU:HD23	3:I:141:ILE:HD13	1.96	0.48
5:Y:277:ASP:HA	5:Y:278:LYS:HA	1.60	0.48
1:A:1268:LYS:O	1:A:1269:HIS:ND1	2.46	0.48
3:G:143:GLN:NE2	5:Y:461:ASN:OD1	2.41	0.48
4:P:40:ARG:NH1	4:P:41:ALA:O	2.46	0.48
1:A:1053:ILE:HG22	1:A:1057:HIS:CE1	2.49	0.48
2:C:296:LYS:HD2	2:C:396:ALA:HB3	1.95	0.48
2:C:853:ASP:OD1	2:C:853:ASP:N	2.46	0.48
2:C:1225:ARG:HH21	2:C:1229:SER:HB2	1.78	0.48
4:P:293:LEU:HD13	4:P:314:GLN:HA	1.95	0.48
1:A:851:ARG:HH11	1:A:975:TYR:HD1	1.60	0.47
2:C:419:PHE:HB2	2:C:1073:ARG:HG2	1.96	0.47
2:C:1049:LYS:HG3	2:C:1051:THR:HG22	1.95	0.47
4:P:43:LEU:HD12	4:P:46:ILE:HD11	1.96	0.47
4:R:279:THR:OG1	4:R:280:SER:N	2.45	0.47
5:Y:197:GLU:O	5:Y:326:ARG:NH1	2.43	0.47
5:Y:218:SER:HA	5:Y:219:ARG:HA	1.65	0.47
2:C:245:MET:HB2	2:C:1133:ALA:HB2	1.94	0.47
1:A:212:PRO:HA	1:A:215:LYS:HE3	1.96	0.47
1:A:745:ASP:O	1:A:830:LYS:NZ	2.47	0.47
1:A:1217:TYR:CZ	1:A:1222:CYS:HB2	2.49	0.47
1:A:1317:ALA:HA	1:A:1341:GLN:HA	1.97	0.47
2:C:244:PHE:HZ	2:C:255:ILE:HA	1.79	0.47
3:G:115:LEU:HB2	3:G:141:ILE:HD13	1.97	0.47
3:I:11:LEU:HA	3:I:82:LYS:HD3	1.96	0.47
4:R:113:ILE:HD11	4:R:295:VAL:HG23	1.96	0.47
1:A:279:ASN:OD1	1:A:282:GLY:N	2.46	0.47
1:A:603:CYS:SG	1:A:608:ARG:NE	2.83	0.47
2:C:203:LYS:HZ1	2:C:1126:THR:H	1.62	0.47
2:C:559:LEU:HB3	2:C:1270:SER:HA	1.96	0.47
4:P:278:SER:O	4:P:280:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:116:LEU:HD12	5:Y:179:CYS:HB2	1.97	0.47
5:Y:129:SER:HA	5:Y:289:PRO:HD2	1.97	0.47
5:d:77:VAL:HG22	5:d:78:ILE:H	1.79	0.47
1:A:1227:ARG:HE	1:A:1245:MET:HA	1.79	0.47
2:C:241:ASP:N	2:C:241:ASP:OD1	2.45	0.47
2:C:599:PRO:HD2	2:C:602:LEU:HD23	1.96	0.47
2:C:633:THR:HG21	2:C:678:VAL:HG12	1.97	0.47
2:C:851:ARG:NH2	2:C:971:GLY:O	2.44	0.47
4:P:37:LEU:HD12	5:Y:307:LEU:HD22	1.96	0.47
4:P:291:ALA:H	4:P:292:ILE:HG23	1.80	0.47
1:A:1357:SER:HG	1:A:1380:TYR:H	1.63	0.47
2:C:441:PHE:HE1	2:C:1361:MET:HG3	1.80	0.47
2:C:461:ASN:HA	2:C:1141:MET:HB2	1.96	0.47
2:C:687:LEU:HA	2:C:690:ILE:HD12	1.96	0.47
2:C:1258:ARG:HH22	2:C:1261:LEU:HA	1.79	0.47
3:I:277:ILE:H	3:I:278:SER:HB3	1.78	0.47
3:I:127:ARG:NH1	3:I:128:LEU:O	2.48	0.47
5:Y:292:VAL:HA	5:Y:293:PHE:HA	1.74	0.47
2:C:864:VAL:HB	2:C:910:LEU:HD22	1.96	0.47
2:C:969:ALA:O	2:C:972:THR:OG1	2.33	0.47
3:I:53:ILE:HA	3:I:54:ASN:HA	1.67	0.47
1:A:846:CYS:HA	1:A:983:PHE:HB3	1.97	0.46
2:C:499:ASP:OD1	2:C:499:ASP:N	2.47	0.46
5:d:426:GLY:HA2	5:d:457:TRP:HA	1.97	0.46
1:A:1144:THR:OG1	1:A:1202:SER:O	2.32	0.46
2:C:461:ASN:OD1	2:C:462:LYS:N	2.47	0.46
2:C:475:MET:HB3	2:C:1059:LEU:HD21	1.97	0.46
2:C:849:GLY:N	2:C:975:TYR:O	2.38	0.46
4:R:266:ARG:H	4:R:267:PHE:HA	1.79	0.46
5:Y:329:LEU:HD11	5:Y:425:ILE:HG21	1.97	0.46
1:A:498:LEU:HB3	1:A:585:PRO:HG2	1.97	0.46
1:A:789:MET:HE1	1:A:917:MET:HE3	1.96	0.46
1:A:724:PHE:HA	1:A:1061:THR:HG21	1.97	0.46
2:C:385:VAL:HG21	2:C:394:LEU:HD13	1.97	0.46
4:R:262:ASP:HB3	5:d:150:PRO:HG3	1.95	0.46
1:A:225:VAL:HG21	2:C:1200:GLN:HG2	1.98	0.46
2:C:416:ASP:HA	2:C:1075:ASP:O	2.15	0.46
2:C:725:THR:HB	2:C:740:ASN:HD22	1.81	0.46
1:A:1097:ILE:HD11	1:A:1112:LEU:HD12	1.97	0.46
1:A:460:TYR:HB3	1:A:464:GLY:HA2	1.98	0.46
1:A:1164:GLU:OE1	1:A:1168:ARG:NE	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1171:ALA:O	1:A:1177:ASN:ND2	2.48	0.46
2:C:553:PRO:HA	2:C:556:ARG:HH12	1.80	0.46
3:I:25:GLN:HA	3:I:78:VAL:HG21	1.97	0.46
4:P:292:ILE:HG13	4:P:293:LEU:HD23	1.98	0.46
1:A:502:CYS:SG	1:A:503:TYR:N	2.89	0.46
2:C:623:THR:O	2:C:626:THR:OG1	2.30	0.46
3:G:296:CYS:HB3	3:G:313:ILE:HD12	1.96	0.46
1:A:67:ASP:N	1:A:67:ASP:OD1	2.49	0.46
2:C:453:PRO:HD3	2:C:610:CYS:HB3	1.98	0.45
3:G:190:VAL:HG22	3:G:191:GLN:H	1.81	0.45
1:A:461:ASN:HA	1:A:1141:MET:HB2	1.98	0.45
1:A:640:PRO:HD2	1:A:643:PHE:HE2	1.81	0.45
2:C:621:THR:OG1	2:C:1037:ASN:OD1	2.34	0.45
2:C:633:THR:HA	2:C:677:ARG:HD3	1.98	0.45
3:I:208:MET:HG2	4:R:225:LEU:HD11	1.98	0.45
3:I:213:GLU:HG3	4:R:245:VAL:HG22	1.98	0.45
4:R:20:GLU:HA	4:R:126:ILE:HG21	1.99	0.45
5:d:187:LEU:HD11	5:d:327:LEU:HD11	1.99	0.45
2:C:1099:VAL:HG12	2:C:1112:LEU:HG	1.98	0.45
2:C:209:LEU:HD13	2:C:234:LEU:HD12	1.98	0.45
2:C:681:VAL:O	2:C:832:TYR:OH	2.35	0.45
3:G:108:CYS:SG	5:Y:113:GLN:NE2	2.78	0.45
3:G:220:ALA:HA	3:G:221:LEU:HA	1.64	0.45
3:I:190:VAL:HG13	3:I:192:GLN:H	1.81	0.45
4:P:114:CYS:HB2	4:P:141:ILE:HG23	1.97	0.45
4:R:99:ILE:HG21	4:R:293:LEU:HD11	1.99	0.45
1:A:223:ASN:OD1	1:A:224:ARG:N	2.47	0.45
1:A:531:MET:HE3	1:A:532:PRO:HD2	1.97	0.45
3:I:277:ILE:HG13	4:R:151:ALA:HB3	1.98	0.45
4:R:89:GLY:HA2	4:R:292:ILE:HD11	1.98	0.45
2:C:1010:PRO:HG2	2:C:1013:LEU:HB2	1.98	0.45
4:P:266:ARG:H	4:P:267:PHE:HA	1.82	0.45
5:d:132:LEU:HD13	5:d:247:PHE:HA	1.98	0.45
3:I:142:PRO:HD2	3:I:145:LEU:HD22	1.98	0.45
3:I:220:ALA:HA	3:I:221:LEU:HA	1.53	0.45
1:A:773:ILE:HG23	1:A:780:GLY:H	1.81	0.45
2:C:548:ILE:HD13	2:C:1258:ARG:HH21	1.81	0.45
3:I:174:LEU:HD22	4:R:270:TYR:HD2	1.81	0.45
2:C:683:ASN:OD1	2:C:754:TRP:NE1	2.50	0.45
3:G:119:VAL:HG12	3:G:120:PHE:H	1.82	0.45
3:I:313:ILE:HD13	5:d:109:GLN:HE22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:252:LEU:N	5:Y:264:THR:O	2.49	0.45
5:d:270:PRO:HB3	5:d:456:VAL:HG22	1.98	0.45
4:R:24:LEU:HD21	4:R:83:LEU:HD13	1.98	0.44
1:A:660:LEU:HD22	1:A:663:LEU:HD21	1.99	0.44
1:A:769:ARG:NH2	1:A:934:ASP:OD2	2.49	0.44
1:A:1094:VAL:HA	1:A:1116:ARG:HD2	1.98	0.44
5:d:22:ALA:HB1	5:d:23:ALA:HA	1.98	0.44
5:d:117:THR:OG1	5:d:259:ASN:OD1	2.36	0.44
5:d:141:PRO:HG2	5:d:158:ALA:HB2	1.98	0.44
1:A:663:LEU:HB3	1:A:909:ALA:HB1	2.00	0.44
2:C:95:LYS:HD2	2:C:95:LYS:HA	1.85	0.44
3:I:117:PRO:HA	3:I:139:LEU:HD11	1.99	0.44
4:R:36:THR:OG1	4:R:38:ARG:NH2	2.40	0.44
5:Y:206:ALA:HB1	5:Y:447:VAL:HG22	2.00	0.44
1:A:163:THR:OG1	1:A:164:GLU:N	2.49	0.44
1:A:247:ARG:NH1	1:A:1387:PRO:O	2.51	0.44
1:A:785:HIS:HB3	1:A:803:HIS:HB3	1.98	0.44
1:A:1058:GLN:NE2	1:A:1059:LEU:HG	2.32	0.44
3:G:99:ILE:HG12	3:G:312:VAL:HG11	1.98	0.44
5:Y:181:ARG:HA	5:Y:182:ALA:HA	1.70	0.44
1:A:908:ASP:OD1	1:A:908:ASP:N	2.50	0.44
1:A:752:ILE:HD11	1:A:957:ILE:HG13	2.00	0.44
3:G:98:PHE:HB3	3:G:311:ALA:HA	2.00	0.44
3:G:146:MET:O	3:G:147:ARG:HG3	2.18	0.44
4:P:241:THR:OG1	4:P:242:ALA:N	2.51	0.44
1:A:796:ARG:NE	1:A:922:GLU:OE2	2.51	0.44
1:A:1035:ASP:HB3	1:A:1038:THR:HG22	2.00	0.44
2:C:597:ASN:ND2	2:C:1022:ARG:HE	2.16	0.44
2:C:686:MET:O	2:C:689:TYR:HB2	2.18	0.44
2:C:939:THR:N	2:C:942:THR:OG1	2.51	0.44
4:P:99:ILE:N	4:P:309:ARG:HH22	2.15	0.44
4:R:278:SER:O	4:R:280:SER:N	2.50	0.44
5:d:426:GLY:HA2	5:d:458:GLY:H	1.81	0.44
2:C:688:MET:SD	2:C:688:MET:N	2.91	0.44
5:Y:133:ILE:HB	5:Y:248:PHE:HB2	2.00	0.44
2:C:781:TYR:HA	2:C:799:ASN:HD22	1.82	0.43
2:C:980:ASN:HB3	2:C:983:PHE:H	1.83	0.43
2:C:1152:ARG:NH2	2:C:1186:GLY:O	2.51	0.43
3:I:20:GLU:HB3	3:I:128:LEU:HD13	1.99	0.43
3:I:90:VAL:HG12	4:R:313:ILE:HG21	2.00	0.43
4:R:45:ASP:OD2	4:R:50:SER:OG	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:210:SER:O	4:R:215:THR:OG1	2.35	0.43
5:d:307:LEU:HG	5:d:429:PRO:HB3	2.00	0.43
1:A:646:LEU:HA	1:A:649:VAL:HG22	2.00	0.43
1:A:1352:PRO:HD2	1:A:1385:ALA:HB3	2.01	0.43
2:C:864:VAL:HG23	2:C:883:PRO:HG3	2.00	0.43
3:G:53:ILE:HA	3:G:54:ASN:HA	1.78	0.43
3:G:98:PHE:HA	3:G:312:VAL:HG13	1.99	0.43
5:Y:130:THR:HG23	5:Y:187:LEU:HB3	2.00	0.43
2:C:1081:GLN:HA	2:C:1131:THR:HA	2.00	0.43
5:d:200:ASP:OD1	5:d:200:ASP:N	2.49	0.43
5:d:324:GLY:HA2	5:d:325:VAL:HA	1.74	0.43
1:A:547:PHE:HE1	1:A:554:ARG:HG3	1.83	0.43
5:d:30:ALA:HA	5:d:31:ALA:HA	1.73	0.43
2:C:1095:GLY:H	2:C:1116:ARG:HH21	1.67	0.43
4:P:173:GLY:HA2	4:P:174:ALA:HA	1.68	0.43
4:R:109:ASN:HA	4:R:295:VAL:HG11	2.00	0.43
1:A:139:ARG:HB3	1:A:1116:ARG:O	2.18	0.43
1:A:962:GLN:HE22	1:A:964:TYR:HB2	1.82	0.43
2:C:135:ARG:HG2	2:C:136:ILE:H	1.84	0.43
2:C:1217:TYR:CZ	2:C:1222:CYS:HB2	2.54	0.43
4:P:279:THR:OG1	4:P:280:SER:N	2.51	0.43
4:R:33:THR:HG23	4:R:70:ARG:HH11	1.84	0.43
1:A:1100:HIS:CE1	1:A:1102:HIS:HB2	2.54	0.43
2:C:161:ASP:N	2:C:161:ASP:OD1	2.51	0.43
5:d:338:CYS:O	5:d:422:TYR:OH	2.33	0.43
1:A:196:LEU:HA	1:A:199:VAL:HG12	2.01	0.43
2:C:263:VAL:O	2:C:390:LYS:NZ	2.48	0.43
1:A:263:VAL:HG11	1:A:387:VAL:HG13	2.01	0.43
3:G:221:LEU:HD23	3:G:226:LEU:HD11	2.00	0.43
5:Y:123:ASP:N	5:Y:123:ASP:OD1	2.52	0.43
5:Y:345:PHE:O	5:Y:347:LEU:N	2.52	0.43
1:A:527:TRP:HA	1:A:530:MET:HG3	2.00	0.42
4:P:259:ARG:HD2	4:P:259:ARG:HA	1.78	0.42
5:d:223:ARG:O	5:d:226:ARG:NH1	2.52	0.42
1:A:209:LEU:HA	1:A:234:LEU:HD11	2.01	0.42
3:G:147:ARG:HH12	5:Y:243:ARG:HD3	1.84	0.42
4:R:45:ASP:OD2	4:R:70:ARG:NH2	2.42	0.42
1:A:421:MET:HE1	1:A:1382:ILE:HG21	2.01	0.42
1:A:1017:HIS:CE1	1:A:1022:ARG:HH12	2.37	0.42
3:G:109:ASN:HD21	3:G:294:ARG:HH21	1.66	0.42
1:A:789:MET:O	1:A:792:HIS:ND1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:922:GLU:HG3	2:C:923:ARG:HD3	2.01	0.42
2:C:1384:ASP:OD1	2:C:1386:SER:OG	2.35	0.42
3:G:201:ARG:HA	3:G:204:VAL:HG12	2.00	0.42
4:P:52:TYR:HA	4:P:58:PRO:HG3	2.02	0.42
1:A:384:LEU:HB3	1:A:391:LEU:HD11	2.01	0.42
1:A:1356:SER:HB3	1:A:1362:LEU:HD12	2.00	0.42
2:C:87:LEU:HG	2:C:196:LEU:HD23	2.01	0.42
1:A:199:VAL:HG22	1:A:203:LYS:HZ2	1.84	0.42
1:A:276:THR:OG1	1:A:277:HIS:N	2.52	0.42
2:C:1227:ARG:NH2	2:C:1247:ASP:O	2.50	0.42
2:C:1267:GLN:HB2	2:C:1270:SER:HB3	2.01	0.42
1:A:423:MET:HE1	1:A:469:LEU:HB3	2.00	0.42
2:C:1257:ASP:N	2:C:1257:ASP:OD2	2.52	0.42
3:G:109:ASN:OD1	3:G:294:ARG:NE	2.52	0.42
3:G:142:PRO:HD2	3:G:145:LEU:HD12	2.01	0.42
5:Y:121:ARG:HA	5:Y:122:PRO:HD3	1.89	0.42
1:A:219:GLU:O	2:C:406:ARG:NE	2.53	0.42
1:A:1049:LYS:HB3	1:A:1051:THR:HG22	2.02	0.42
2:C:980:ASN:ND2	2:C:982:LEU:HB2	2.35	0.42
3:I:28:GLU:HG3	3:I:78:VAL:HB	2.02	0.42
2:C:502:CYS:SG	2:C:503:TYR:N	2.93	0.42
2:C:895:ASN:HD21	2:C:910:LEU:HD11	1.85	0.42
2:C:926:ALA:HB1	2:C:1013:LEU:HD21	2.01	0.42
4:R:52:TYR:HA	4:R:58:PRO:HG3	2.02	0.42
2:C:1095:GLY:O	2:C:1114:GLN:NE2	2.49	0.41
4:R:22:SER:HA	4:R:25:GLN:HG3	2.01	0.41
5:d:181:ARG:HA	5:d:182:ALA:HA	1.77	0.41
1:A:721:ILE:HG12	1:A:743:LEU:HD11	2.00	0.41
2:C:473:ASP:OD1	2:C:474:ALA:N	2.53	0.41
2:C:1200:GLN:HE21	2:C:1329:GLN:HG3	1.85	0.41
3:I:205:LEU:HD21	4:R:235:VAL:HG22	2.02	0.41
4:P:12:LEU:HD21	4:P:16:ILE:HD12	2.02	0.41
4:P:281:SER:O	4:P:282:ARG:HD3	2.20	0.41
5:d:299:ASP:HA	5:d:300:LEU:HB2	2.01	0.41
1:A:205:PRO:HB3	1:A:1312:LEU:HD21	2.02	0.41
1:A:1058:GLN:HB2	1:A:1063:PHE:HB3	2.01	0.41
1:A:1155:VAL:HA	1:A:1156:PRO:HD3	1.91	0.41
2:C:683:ASN:HB3	2:C:686:MET:HE2	2.02	0.41
4:R:193:ARG:O	4:R:197:ASP:N	2.51	0.41
5:Y:335:ASN:H	5:Y:338:CYS:HB2	1.86	0.41
1:A:219:GLU:HB2	2:C:406:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:846:CYS:HB2	2:C:985:CYS:HB3	1.41	0.41
3:G:48:LEU:HD13	3:G:136:VAL:HG21	2.01	0.41
3:I:17:SER:OG	3:I:20:GLU:OE1	2.36	0.41
4:P:128:LEU:HG	4:P:131:VAL:HG22	2.03	0.41
4:P:236:ASN:HA	4:P:237:LEU:HA	1.82	0.41
2:C:1209:MET:SD	2:C:1209:MET:N	2.93	0.41
4:P:52:TYR:HD1	4:P:58:PRO:HD3	1.85	0.41
5:d:184:VAL:HG21	5:d:263:ILE:HD11	2.02	0.41
1:A:1152:ARG:HG3	4:P:233:GLY:HA2	2.02	0.41
2:C:726:ILE:HD12	2:C:1060:ARG:HD2	2.02	0.41
2:C:778:ARG:NH1	2:C:798:ASP:HA	2.36	0.41
2:C:1069:PHE:HA	2:C:1207:VAL:O	2.21	0.41
3:I:304:VAL:HG22	3:I:310:THR:HG21	2.02	0.41
4:R:146:MET:HE3	4:R:150:ILE:HD11	2.02	0.41
5:Y:324:GLY:HA2	5:Y:325:VAL:HA	1.78	0.41
1:A:145:PHE:HD2	1:A:1110:PHE:HB2	1.86	0.41
1:A:721:ILE:HD12	1:A:721:ILE:HA	1.85	0.41
2:C:308:ASP:H	2:C:384:LEU:HB2	1.86	0.41
2:C:1013:LEU:HD23	2:C:1013:LEU:HA	1.88	0.41
5:Y:133:ILE:N	5:Y:246:SER:O	2.53	0.41
1:A:136:ILE:HA	1:A:1119:VAL:HG22	2.03	0.41
1:A:251:GLU:HA	1:A:252:PRO:HD3	1.91	0.41
1:A:259:LEU:HA	1:A:262:MET:HG3	2.01	0.41
1:A:828:LEU:HA	1:A:831:ILE:HG12	2.01	0.41
3:I:148:GLU:HB3	3:I:152:LYS:NZ	2.36	0.41
1:A:379:ARG:HD3	1:A:379:ARG:HA	1.89	0.41
1:A:507:TYR:OH	1:A:577:PRO:O	2.33	0.41
1:A:1072:VAL:HG11	1:A:1292:CYS:HB3	2.02	0.41
1:A:1146:GLN:HE22	1:A:1288:ILE:HG23	1.86	0.41
1:A:1225:ARG:NH2	1:A:1227:ARG:O	2.54	0.41
3:G:187:VAL:HG13	3:G:193:LEU:HD13	2.02	0.41
5:Y:108:THR:HG22	5:Y:266:VAL:HG21	2.03	0.41
5:Y:316:TYR:HA	5:Y:325:VAL:HG22	2.03	0.41
5:d:20:ALA:H	5:d:22:ALA:HB3	1.86	0.41
1:A:478:ILE:HB	1:A:1069:PHE:HZ	1.86	0.41
2:C:1163:THR:HG22	2:C:1167:ARG:HH21	1.86	0.41
3:G:213:GLU:HG2	4:P:245:VAL:HG13	2.03	0.41
3:I:113:ILE:HD13	3:I:289:THR:H	1.86	0.41
4:P:29:GLY:O	4:P:100:GLN:N	2.38	0.41
1:A:764:GLU:O	1:A:767:ARG:NH2	2.54	0.40
1:A:933:PRO:HG3	1:A:942:THR:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:225:LEU:HD23	3:I:226:LEU:HD12	2.03	0.40
3:I:294:ARG:HH11	3:I:295:VAL:H	1.69	0.40
4:R:148:GLU:O	4:R:152:LYS:NZ	2.39	0.40
4:R:173:GLY:HA2	4:R:174:ALA:HA	1.79	0.40
2:C:877:PRO:HA	2:C:882:HIS:CG	2.56	0.40
4:P:10:VAL:HB	4:P:83:LEU:HG	2.02	0.40
4:P:52:TYR:HD1	4:P:57:PRO:HA	1.86	0.40
5:d:193:CYS:SG	5:d:228:SER:OG	2.64	0.40
1:A:782:GLN:HB2	1:A:800:VAL:HA	2.03	0.40
2:C:222:LEU:O	2:C:227:ARG:NH2	2.53	0.40
2:C:1240:ASP:O	2:C:1243:ALA:HB3	2.20	0.40
2:C:1357:SER:HB3	2:C:1380:TYR:H	1.87	0.40
3:G:45:ASP:HA	3:G:50:SER:HB3	2.04	0.40
1:A:594:ILE:HG22	1:A:596:GLY:N	2.37	0.40
2:C:457:ILE:HG22	2:C:469:LEU:HB2	2.02	0.40
2:C:803:HIS:NE2	2:C:818:THR:O	2.46	0.40
4:P:168:PRO:HA	4:P:169:GLY:HA2	1.82	0.40
5:Y:206:ALA:HB1	5:Y:447:VAL:HA	2.03	0.40
5:Y:312:LEU:HD12	5:Y:425:ILE:HD12	2.03	0.40
5:d:277:ASP:HA	5:d:278:LYS:HA	1.65	0.40
2:C:1263:PRO:HA	2:C:1267:GLN:HE22	1.86	0.40
5:d:83:ASN:HA	5:d:84:ILE:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1339/1345 (100%)	1181 (88%)	152 (11%)	6 (0%)	30	67
2	C	1291/1297 (100%)	1180 (91%)	110 (8%)	1 (0%)	48	83
3	G	287/297 (97%)	230 (80%)	49 (17%)	8 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	287/297 (97%)	229 (80%)	49 (17%)	9 (3%)	3	21
4	P	299/307 (97%)	248 (83%)	42 (14%)	9 (3%)	3	22
4	R	299/307 (97%)	254 (85%)	36 (12%)	9 (3%)	3	22
5	Y	283/357 (79%)	238 (84%)	38 (13%)	7 (2%)	4	26
5	d	347/357 (97%)	278 (80%)	53 (15%)	16 (5%)	2	16
All	All	4432/4564 (97%)	3838 (87%)	529 (12%)	65 (2%)	11	38

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	84	GLU
3	G	40	ARG
3	G	98	PHE
3	G	103	SER
3	G	190	VAL
3	I	103	SER
3	I	119	VAL
3	I	190	VAL
4	P	46	ILE
4	P	218	ILE
4	P	269	ILE
4	P	292	ILE
4	R	46	ILE
4	R	218	ILE
4	R	269	ILE
5	Y	141	PRO
5	Y	256	ILE
5	d	30	ALA
5	d	47	ALA
5	d	77	VAL
5	d	141	PRO
5	d	188	SER
5	d	256	ILE
1	A	41	VAL
1	A	42	CYS
2	C	160	VAL
3	I	98	PHE
4	P	45	ASP
4	P	274	SER

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Mol	Chain	Res	Type
4	P	279	THR
4	R	45	ASP
4	R	274	SER
4	R	279	THR
5	d	20	ALA
3	G	84	LEU
4	P	303	THR
4	R	180	ASN
5	Y	254	TYR
5	Y	300	LEU
5	d	48	ALA
5	d	87	ASN
1	A	267	GLN
3	I	84	LEU
5	Y	460	THR
5	d	300	LEU
3	G	126	ILE
3	I	126	ILE
3	I	212	ASN
4	R	235	VAL
5	d	120	PHE
5	d	251	LEU
5	d	254	TYR
5	d	460	THR
3	G	291	ALA
3	I	38	ARG
4	R	303	THR
5	Y	120	PHE
5	Y	251	LEU
5	d	83	ASN
5	d	91	ILE
3	G	153	VAL
3	I	153	VAL
4	P	235	VAL
1	A	54	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1089/1137 (96%)	1087 (100%)	2 (0%)	87	86
2	C	1072/1093 (98%)	1071 (100%)	1 (0%)	88	88
3	G	212/252 (84%)	212 (100%)	0	100	100
3	I	212/252 (84%)	212 (100%)	0	100	100
4	P	242/258 (94%)	242 (100%)	0	100	100
4	R	242/258 (94%)	242 (100%)	0	100	100
5	Y	220/270 (82%)	220 (100%)	0	100	100
5	d	244/270 (90%)	244 (100%)	0	100	100
All	All	3533/3790 (93%)	3530 (100%)	3 (0%)	87	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	267	GLN
2	C	195	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	ASN
1	A	267	GLN
1	A	455	GLN
1	A	501	GLN
1	A	685	HIS
1	A	741	ASN
1	A	900	ASN
1	A	1016	ASN
1	A	1098	GLN
1	A	1143	ASN
1	A	1146	GLN
1	A	1177	ASN
1	A	1216	GLN
2	C	277	HIS
2	C	305	GLN
2	C	427	GLN
2	C	437	HIS

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Mol	Chain	Res	Type
2	C	495	GLN
2	C	501	GLN
2	C	597	ASN
2	C	696	ASN
2	C	895	ASN
2	C	1102	HIS
2	C	1143	ASN
2	C	1159	HIS
3	G	206	ASN
3	I	162	ASN
3	I	175	ASN
4	P	143	GLN
4	P	305	HIS
5	Y	202	GLN
5	Y	236	GLN
5	Y	318	GLN
5	Y	321	GLN
5	Y	333	GLN
5	d	83	ASN
5	d	136	HIS
5	d	242	HIS
5	d	309	HIS
5	d	318	GLN
5	d	328	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	d	4
3	I	4
3	G	4
4	R	3
4	P	3
2	C	2
1	A	2
5	Y	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	45:PHE	C	81:ARG	N	44.28
1	d	36:ALA	C	44:ALA	N	41.89
1	A	360:GLU	C	377:ASN	N	31.99
1	C	338:ARG	C	377:ASN	N	25.70
1	d	51:ALA	C	76:ILE	N	23.55
1	R	250:GLN	C	256:PRO	N	17.10
1	P	250:GLN	C	256:PRO	N	16.91
1	d	351:ILE	C	417:CYS	N	14.16
1	I	164:ASP	C	172:PRO	N	13.97
1	G	164:ASP	C	172:PRO	N	13.45
1	Y	351:ILE	C	417:CYS	N	12.57
1	G	260:MET	C	265:ARG	N	11.96
1	A	316:THR	C	325:VAL	N	11.92
1	I	260:MET	C	265:ARG	N	10.39
1	I	228:LEU	C	233:GLY	N	8.61
1	I	194:ALA	C	196:SER	N	8.48
1	G	228:LEU	C	233:GLY	N	7.82
1	G	194:ALA	C	196:SER	N	7.81
1	d	168:SER	C	176:GLU	N	6.04
1	Y	168:SER	C	176:GLU	N	5.77
1	P	164:GLY	C	166:ARG	N	4.45
1	R	164:GLY	C	166:ARG	N	4.16
1	P	220:THR	C	221:LEU	N	3.30

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	R	220:THR	C	221:LEU	N	3.20

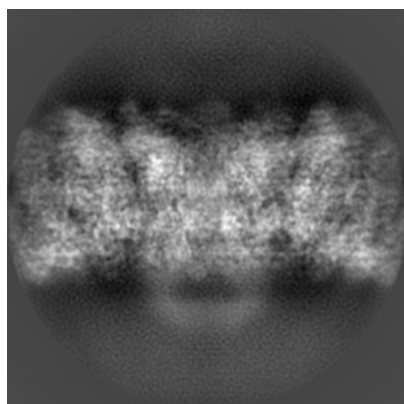
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38191. These allow visual inspection of the internal detail of the map and identification of artifacts.

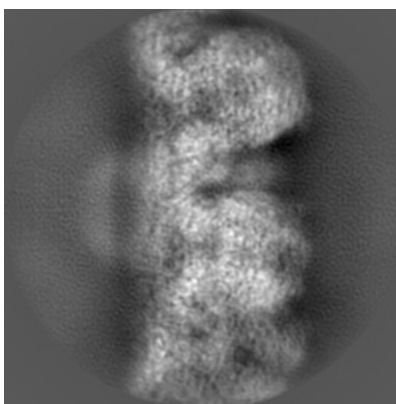
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

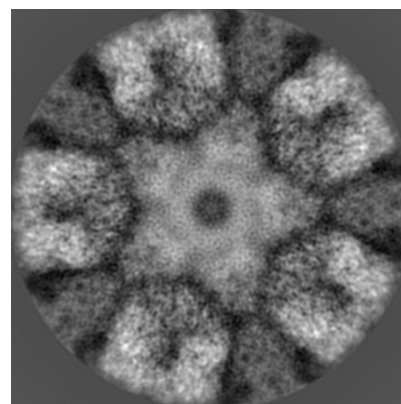
6.1.1 Primary map



X

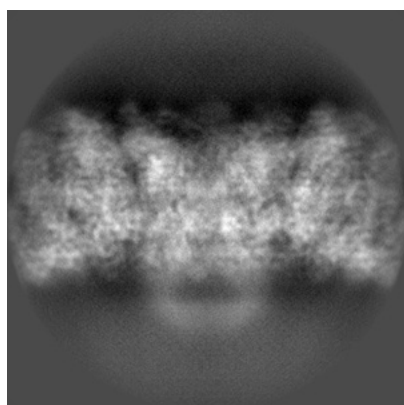


Y

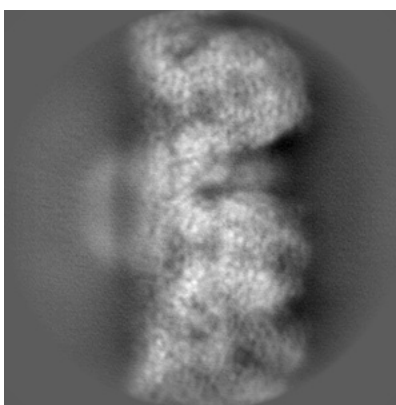


Z

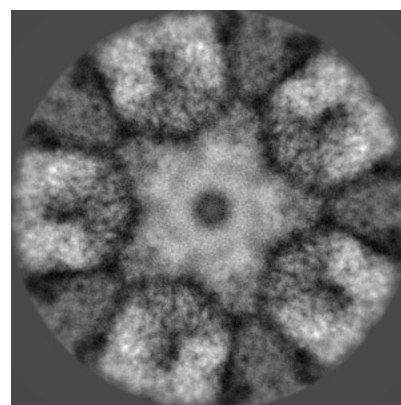
6.1.2 Raw map



X



Y

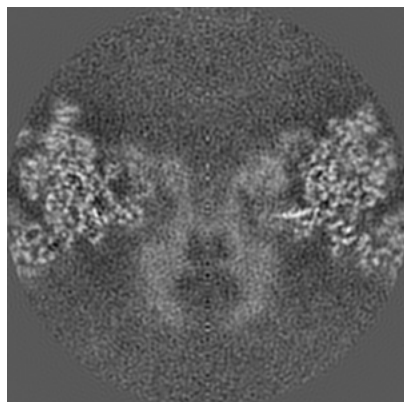


Z

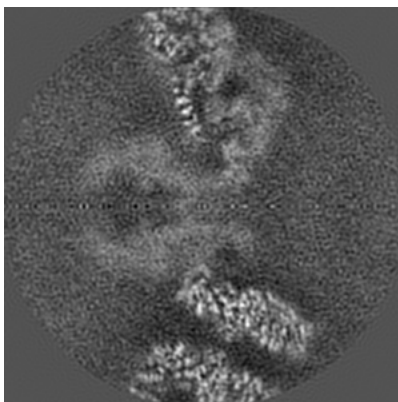
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

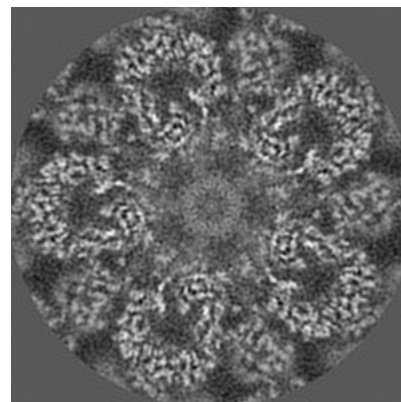
6.2.1 Primary map



X Index: 155

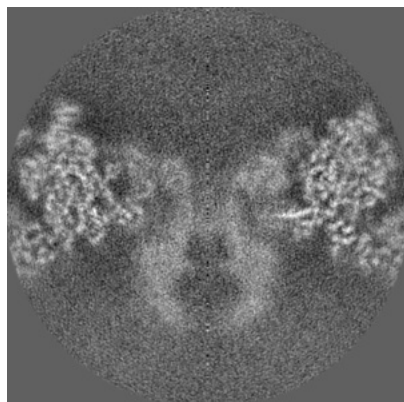


Y Index: 155

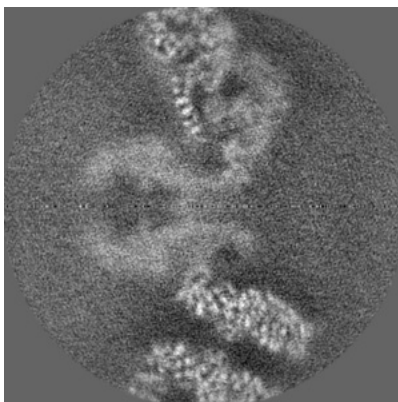


Z Index: 155

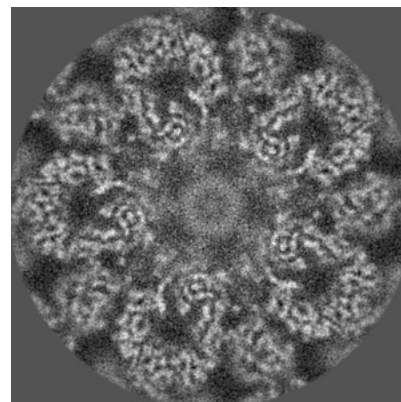
6.2.2 Raw map



X Index: 155



Y Index: 155

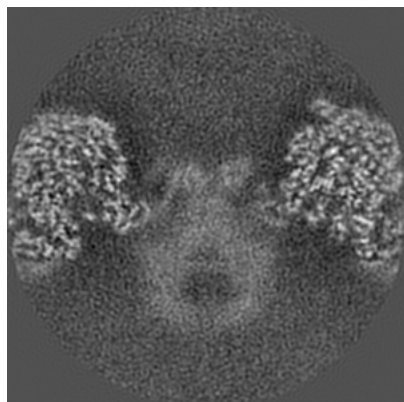


Z Index: 155

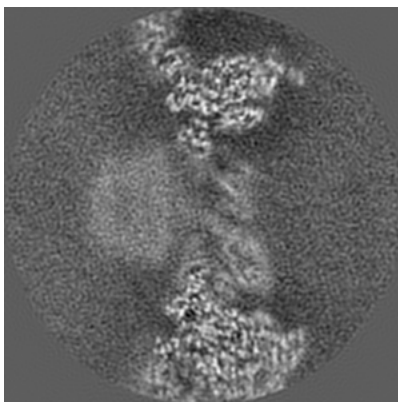
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

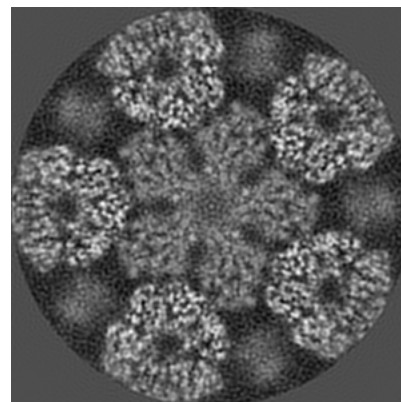
6.3.1 Primary map



X Index: 138

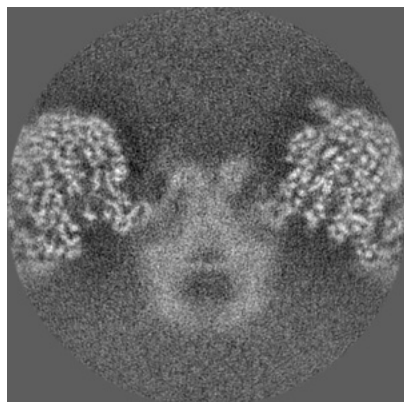


Y Index: 126

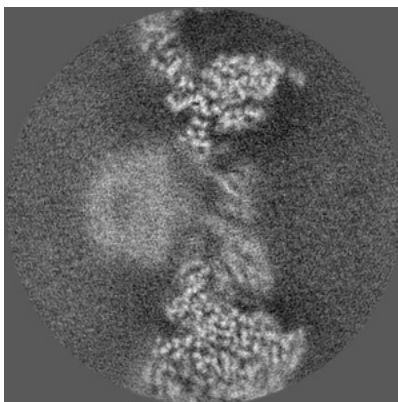


Z Index: 176

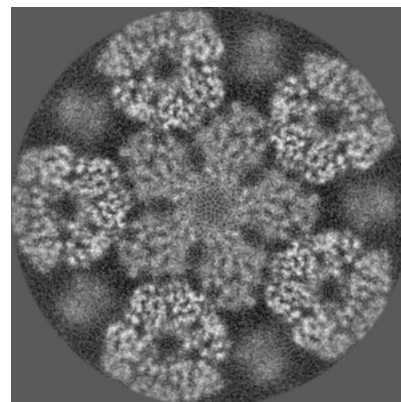
6.3.2 Raw map



X Index: 139



Y Index: 127

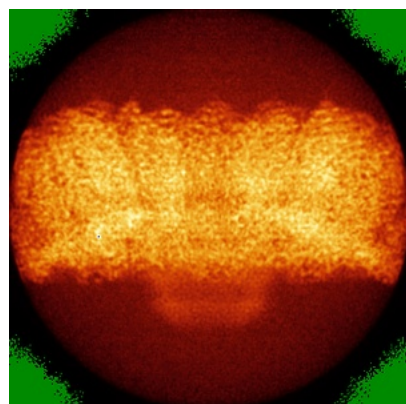


Z Index: 176

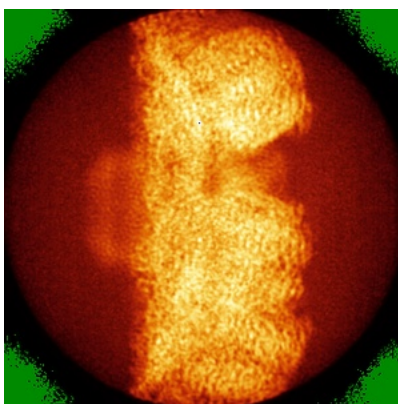
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

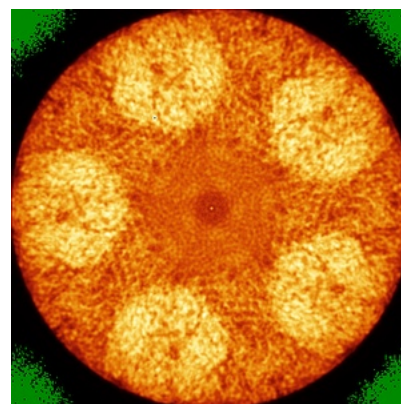
6.4.1 Primary map



X

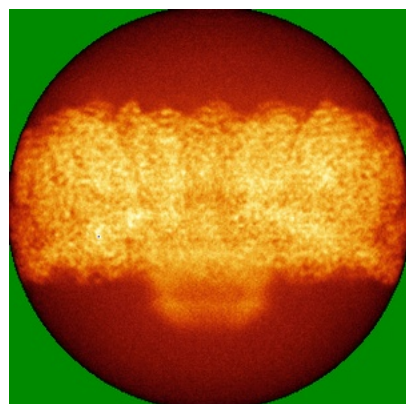


Y

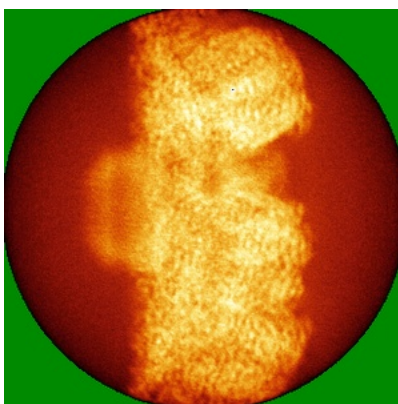


Z

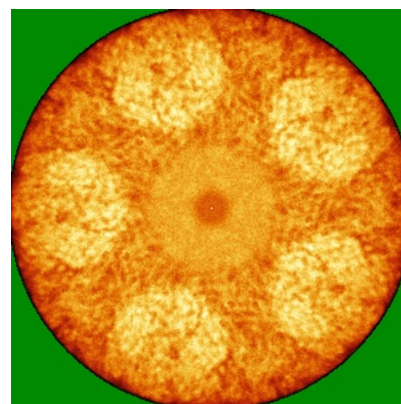
6.4.2 Raw map



X



Y

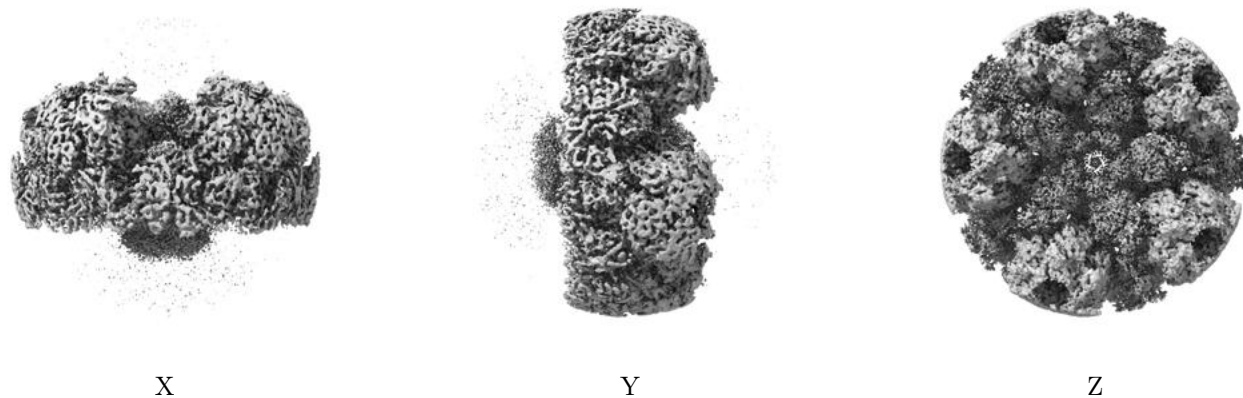


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

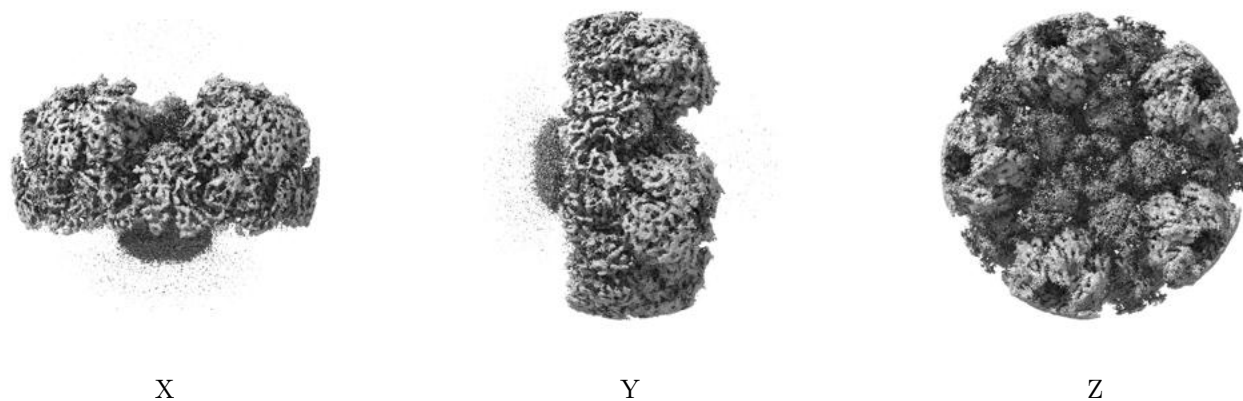
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

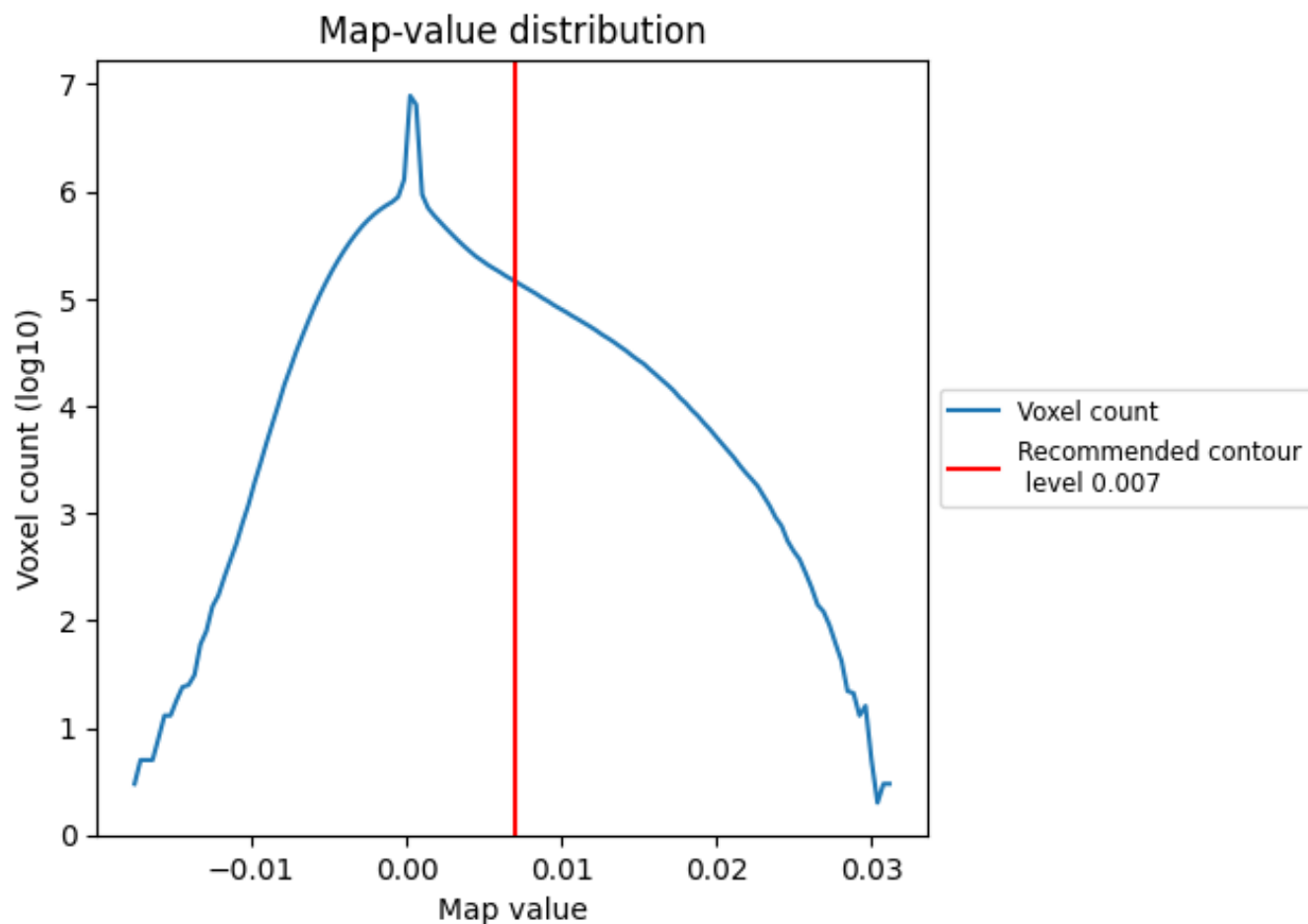
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

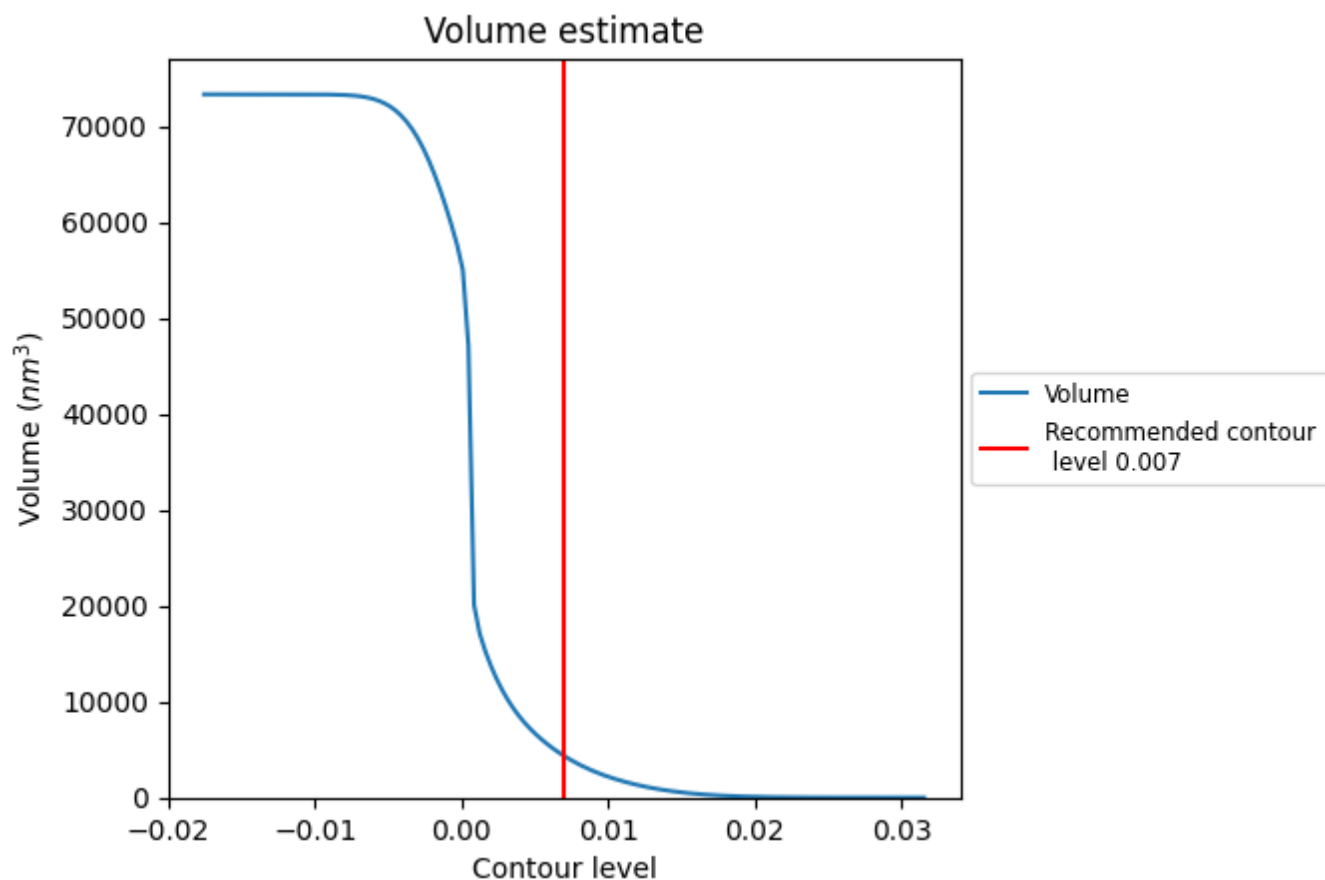
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

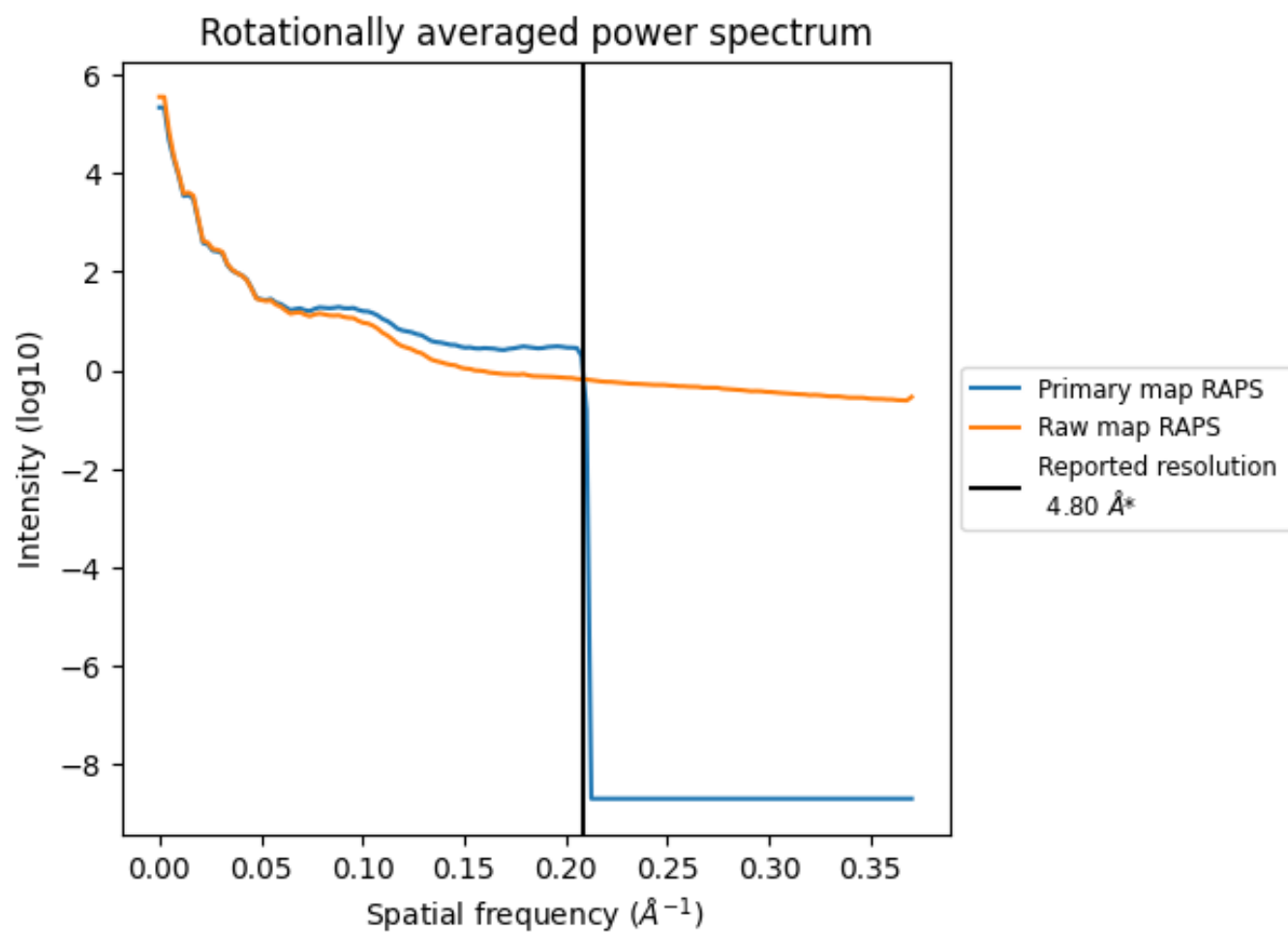
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4343 nm³; this corresponds to an approximate mass of 3924 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

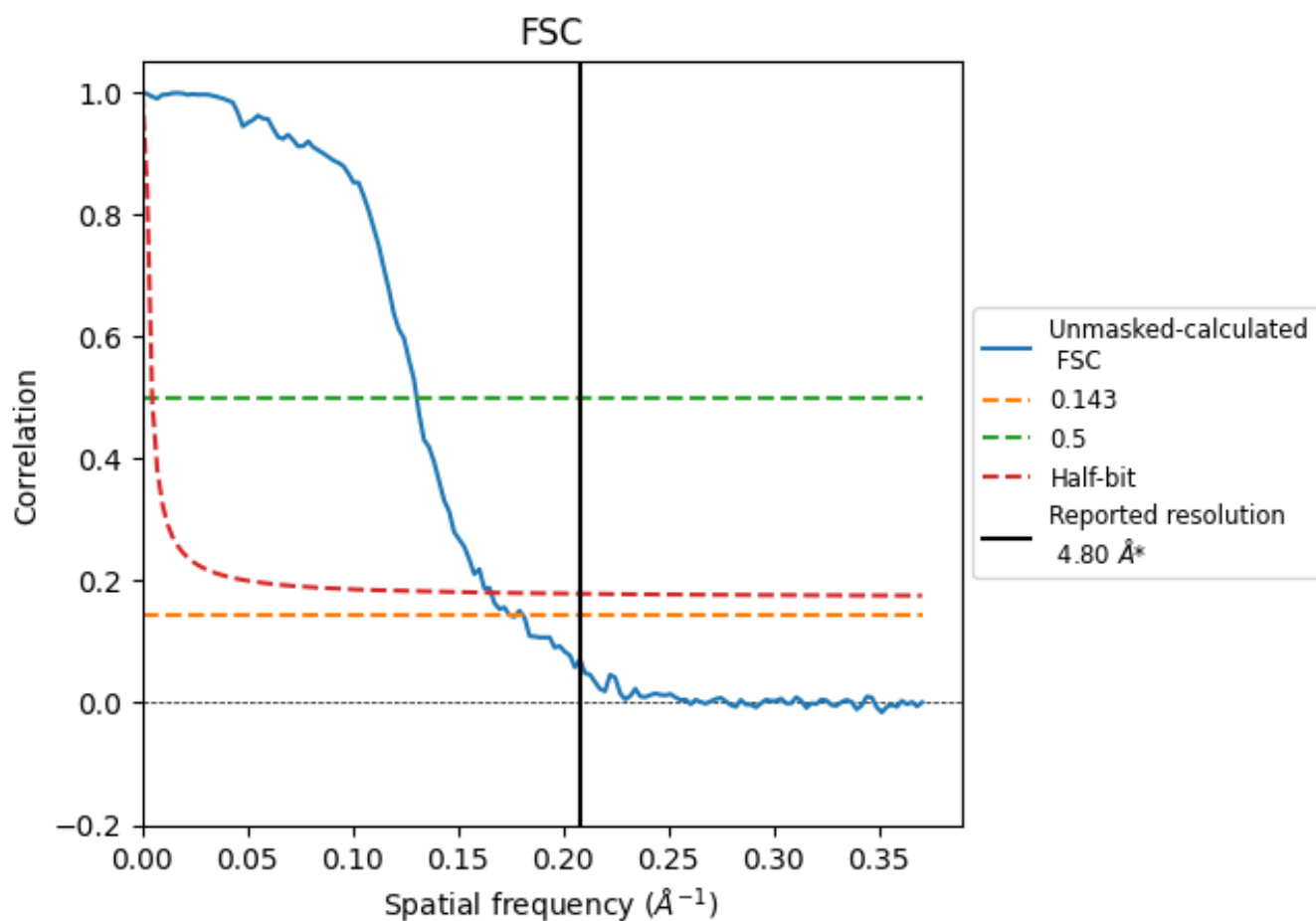


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.72	7.67	6.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.72 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

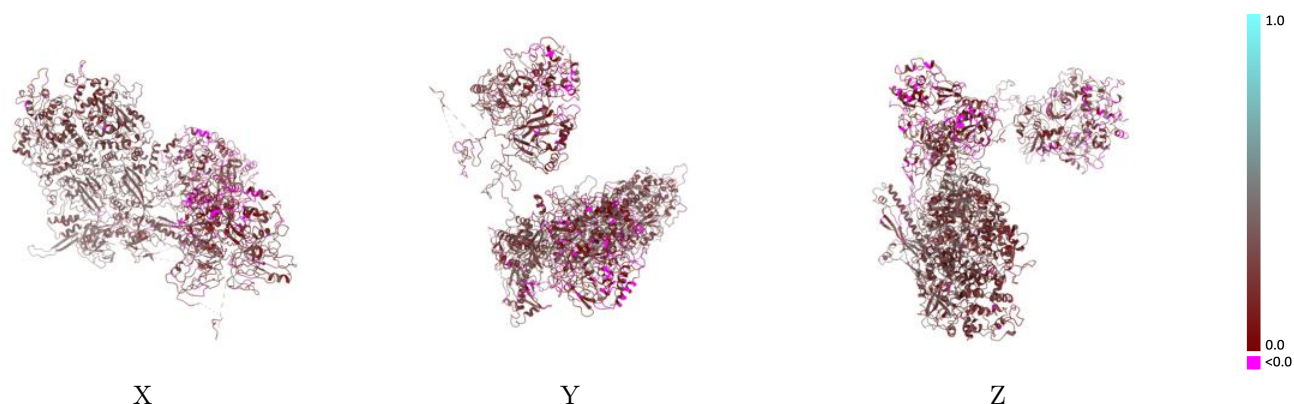
This section contains information regarding the fit between EMDB map EMD-38191 and PDB model 8XA1. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



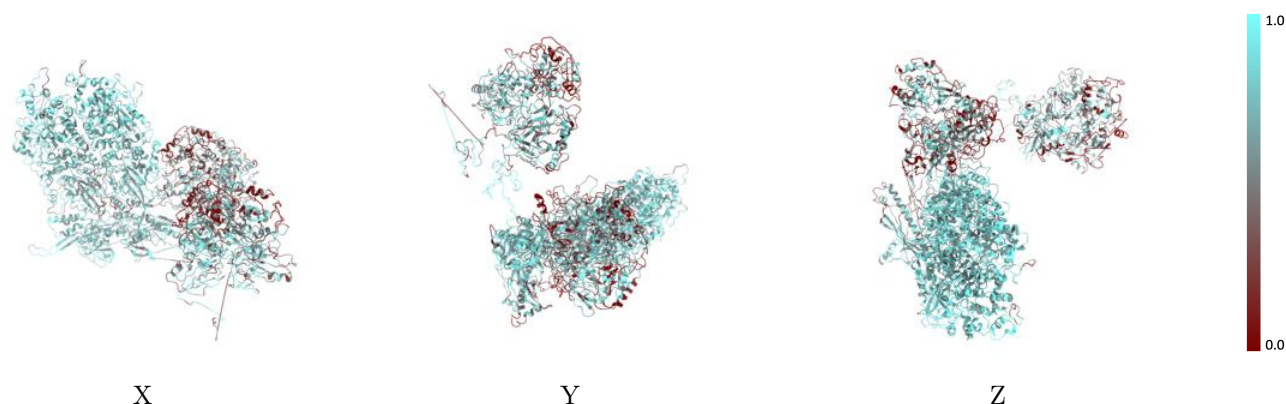
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



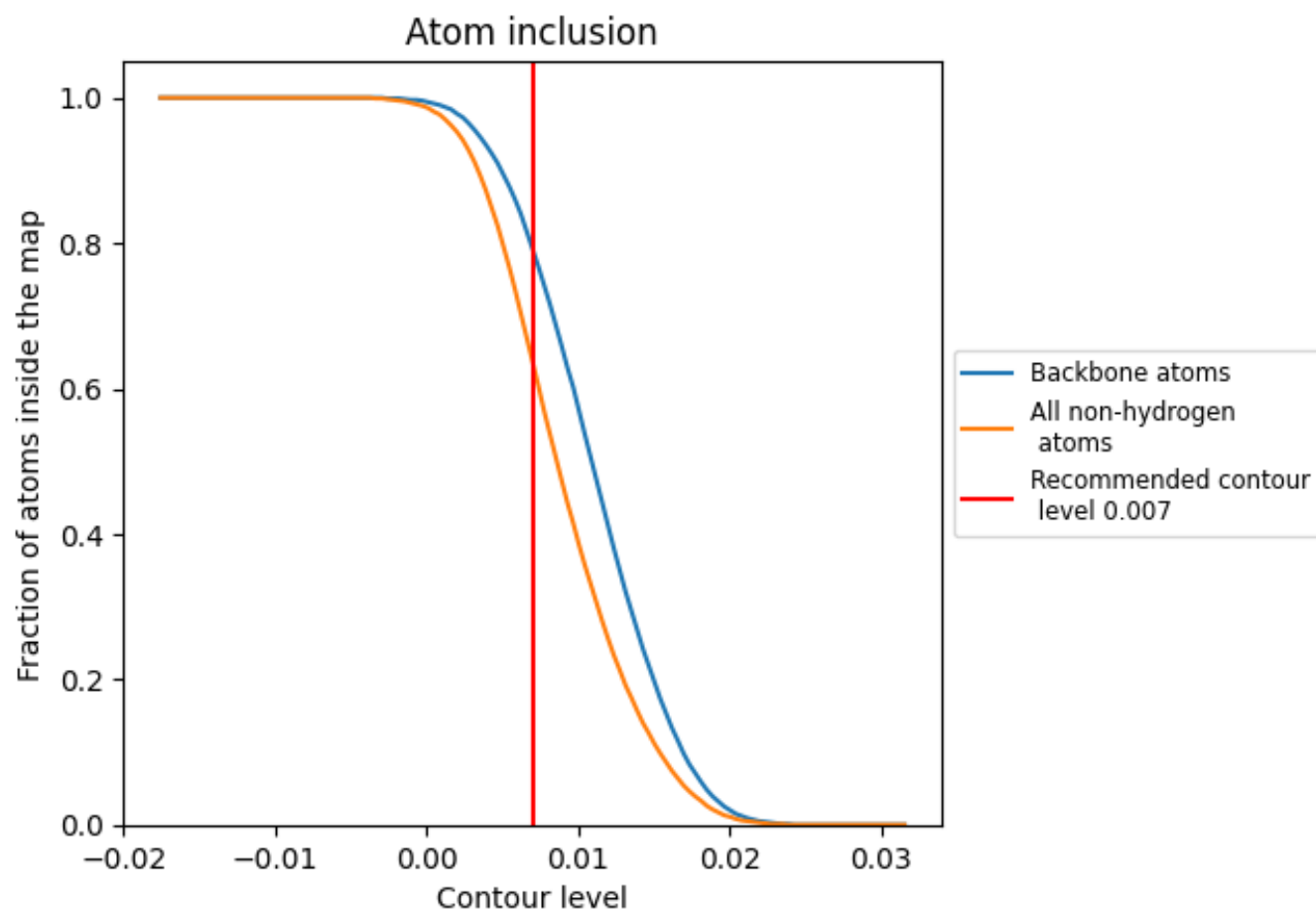
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6360	0.2430
A	0.7390	0.2770
C	0.7440	0.2850
G	0.4630	0.1760
I	0.5380	0.2210
P	0.3390	0.1450
R	0.4610	0.2130
Y	0.5270	0.1500
d	0.5440	0.2070

1.0

0.0

<0.0